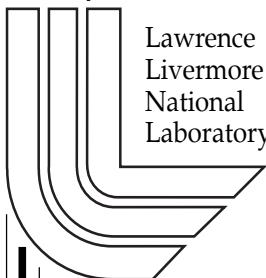


Ab Initio Calculation of Thermodynamic Data for Oxygenated Hydrocarbon Fuels and Radical Breakdown Species: $R(OMe)_n$

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Ab initio Calculation of Thermodynamic Data for Oxygenated Hydrocarbon Fuels and Radical Breakdown Species: R(OMe)_n

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Abstract:

There has long been interest in the use of oxygenated hydrocarbon additives to conventional fuels. These oxygenates have been shown to reduce soot emissions in diesel engines and CO emissions in spark-ignition engines; and often allow diesel operation with decreased NO_x. The current widely used additive, MTBE is targeted for elimination as a gasoline additive due to its damaging effects on the environment. This creates a need for alternative oxygenated additives; and more importantly, amplifies the importance to fully understand the thermochemical and kinetic properties on these oxyhydrocarbons fuels and for their intermediate and radical breakdown products. We use CBS-Q and density-functional methods with isodesmic reactions (with group balance when possible) to compute thermodynamic quantities for these species. We have studied hydrocarbons with multiple substituted methoxy groups. In several cases, multi-oxygenated species are evaluated that may have potential use as new oxygenated fuel additives. Thermodynamic quantities (H^0_{298} , S^0_{298} , $C_p(T)$) as well as group additivity contributions for the new oxygenated groups are reported. We also report trends in bond-energies with increasing methoxy substitution.

Introduction

In recent years, there has been an increased interest in studies of oxygenated additives to diesel and spark-ignition engines, as a result of the elimination of MTBE due to environmental concerns. Alternatives to MTBE, including methanol, ethanol, dimethyl ether and dimethoxymethane have been the focus of recent modeling studies. However, the atmospheric reactivity of these species also plays an important role in the desirability of any fuel additive. There is also interest in the evaluation of other larger oxygenated hydrocarbons, such as trimethoxymethane and tetramethoxymethane, as fuel additives. Some recent modeling efforts[1-4] have focused on the reactivity and environmental impact of various polymethoxyalkane species. Other studies have focused on the experimental and *ab initio* determination of molecular structure and relative energies of various conformations[5-11]. However, to the best of our knowledge, there is very little published data on the thermochemical properties of these

novel species.

In this paper we focus on the thermochemical properties (ΔH_f^0 , S₂₉₈, Cp(T) (for 300 < T/K < 1500) for stable molecules and radical intermediates of the polymethoxyalkane family of molecules using the high-accuracy CBS-Q[13] composite *ab initio* method. The data presented in this study is to enhance the combustion and atmospheric modeling efforts of these, and many other oxygenated hydrocarbon additives. The species of interest here are: tetramethoxymethane, trimethoxymethane, dimethoxymethane, 1,1,1-trimethoxyethane, 1,1-dimethoxyethane, 2,2-dimethoxypropane, and the radical resulting from the removal of a methoxy group from each these stable species.

Nomenclature

The 12 species of interest are represented in Table I as the substitution combinations of hydrogen on methane with the methoxy group, methyl group and a dangling bond. Throughout this paper, we will often refer to these species by shortened notation. Each species is denoted by the following mnemonic, NMAS, or (N)umber of (M)ethoxy (A)lkane (S)pin-multiplicity. N refers to the number of methoxy groups attached to the central carbon, while A specifies the alkane ((M)ethane, (E)thane or (P)ropane). S is either a radical (R), or is left blank, signifying a stable species. For example, 3MM refers to the trimethoxymethane, while 2MER refers to the dimethoxyethyl radical (1,1-dimethoxyethane 1-yl).

Due to the relatively large size and overall floppiness of these polymethoxyalkane molecules, there exist multiple stable conformations which must be properly accounted for in all the thermochemical calculations. With the exception of conformers for 1,1-dimethoxyethane (2ME), each conformation is composed of the same number of letters as there are methoxy groups attached to the central carbon. For 2ME conformers, 3 letters are required. Each letter refers to the relative torsional position of the methyl, on the methoxy group, relative to other carbon(central)-oxygen bonds. These local conformations are denoted according to conventional notation. Synperiplanar (eclipsing), synclinal, anticlinal, antiperiplanar (trans), -synclinal and -anticlinal conformation are given the letters C, G+, A+, T, G-, A- respectively.

Figures 1-12 show the stable conformations of all the species of interest.

Methodology

The procedure for finding the stable conformers of each species involved an initial search at the PM3 semi-empirical level of numerous combinations of C, G+, A+, T, G-, A- conformers. Following this was a refined search with optimizations performed at the B3LYP/6-31G(d,p) level. Total energies for each conformation were calculated at both the B3LYP/6-31G(d,p) and B3LYP/6-311+G(3df,2p) levels, with zero-point vibrational energies (ZPVEs) and standard enthalpy corrections taken from B3LYP/6-31G(d,p) frequency calculations.

The CBS-Q composite *ab initio* method[13] was used, with slight modification, to calculate ΔH_f^0 for each species. For the lowest energy conformation, optimization, SCF energy, 2nd and higher-order correlations and empirical correction terms were taken according to the original CBS-Q method. However, the frequency calculations were performed at the B3LYP/6-31G(d,p) for the B3 optimized conformer. This level was chosen due to the small root-mean-square (rms) error and consequent near-unity correction factors for frequencies, ZPVE and enthalpy correction[13].

To include mixing effects of other conformations on ΔH_f^0 , total and relative energies were calculated for each conformation at the B3LYP/6-311+G(3df,2p)//B3LYP/6-31G(d,p) level. ZPVE values were calculated using B3LYP/6-31G(d,p) frequencies, with scaling corrections from work of Scott and Radom[13]. Contributions of the conformers were included by assuming a Boltzmann distribution.

Isodesmic reactions (with group balance, when possible) were used to calculate ΔH_f^0 . The uncertainty error was taken as the error propagated through the isodesmic reaction. Although there are a number of different possible isodesmic reactions to chose from for each species, we attempted to find the one with the least error propagated. The list of isodesmic reactions used for each species is given in Table II, while the thermochemistry associated with these “isodesmic species” are given in Appendix A. Thermochemistry on polyhydroxyalkane species can be found elsewhere[17].

Calculated and available experimental ΔH_f^0 are given in Table III. The CBS-Q standard enthalpies are given, as well as the B3LYP/6-311+G(3df,2p) and B3LYP/6-31G(d,p) values, for comparison. The uncertainty for the B3LYP/6-311+G(3df,2p) and B3LYP/6-31G(d,p) standard enthalpies are the same as for those for the CBS-Q values.

Evaluation of S_{298} and $C_p(T)$ involved calculating, separately, the contribution from translations, vibrations and external rotations (TVR) and the contribution from hindered internal rotations (IR). The TVR contribution have been calculated for each conformation using the SMCPS[15] software package. Frequencies and rotational constants were calculated at the B3LYP/6-31G(d,p) level, while entropy, frequency and ZPVE correction factors were taken from those suggested by Scott and Radom[13]. Table IV lists the unscaled frequencies for each conformer, while Table V lists the rotational constants.

The IR contributions to S_{298} and $C_p(T)$ from hindered internal rotors were calculated using the method of Lay and coworkers[14]. For each rotor (taken as every bond between two heavy atoms), the potential energy versus dihedral angle surface was calculated through constrained optimization of the molecule for varying dihedral angle at increments of 10 degrees. A potential energy function, $V(\phi)$, was then fit to the calculated data. $V(\phi)$ takes the form of a truncated Fourier series,

$$V(\phi) = a_0 + \sum a_i \cos(j\phi) + b_i \sin(j\phi)$$

Except where noted, the functions were truncated beyond n=6 pairwise terms. A complete list of coefficients for each of the species is given in Appendix B. Energy eigenvalues for rotor motion, used to form the partition function and subsequent entropy and heat capacity contributions, are then calculated by solving the time independent Schrodinger equation, using the software package by Shokhirev and Krasnoperov[16]. Table IV lists S_{298}^0 and $C_p(300 < T/K < 1500)$ according to contributions from the TVRs and IRs for each conformation. In addition, the overall entropy and heat capacity data for the gas-phase equilibrium mixture of conformations is given. The overall heat capacity was calculated assuming a Boltzmann distribution of the conformations relative to a single reference state, taken as the energy of the lowest energy conformation. The overall standard entropy was simply taken as the arithmetic mean, given the small differences in entropy between the conformers.

Discussion of Results

Below we have made brief discussions on the conformations of the stable species in this study. Detailed discussions of the relative stabilities, as well as the geometries can be found elsewhere[17].

Conformations of Stable Species

Tetramethoxymethane

Figure 1 shows the three stable conformations (TTT, $G^+G^-G^+G^-$, and $A^+G^+G^-G^+$) which we have found for tetramethoxymethane. The naming convention of these conformations goes according to the dihedral angle about the central carbon-oxygen bond axis. For example, for the TTT conformation, bond 2-7 is trans to bond 1-3, 3-6 is trans 1-4, 4-9 is trans to 1-5 and 5-8 is trans to 1-2.

The TTT conformation was found to be the most stable, with $A^+G^+G^-G^+$ and $G^+G^-G^+G^-$ at 4.49 kcal/mol and 2.41 kcal/mol higher energy, respectively, relative to TTT. The determination of the TTT conformation as the most stable has been confirmed by electron diffraction experiments of Mulhoff and coworkers, as well as *ab initio* HF/STO-3G calculations of McEachern.

Trimethoxymethane

Figure 2 shows the four stable conformations (TTG⁻, TTT, CCC, G⁻TG⁺ and G⁺TG⁺) found for trimethoxymethane. The most stable conformation is found to be TTG⁻, in agreement with ab initio calculations of Spelbos. We have found the other conformations, TTT, CCC, G⁻TG⁺ and G⁺TG⁺ at 0.42, 8.72, 0.68 and 4.13 kcal/mol, respectively, higher than TTG⁻. These results differ from those of Spelbos, who considered three conformations (TTG⁻, TTT and G⁻TG⁺) with the TTT and G⁻TG⁺ conformations 1.4 and 2.7 kcal/mol, respectively, above the TTG⁻ conformation.

Dimethoxymethane

Figure 3 shows the four stable conformations (TG⁻, TT, G⁺G⁺ and G⁻G⁺). G⁺G⁺ appears as the most stable conformation, in agreement with results from NMR experiments of Abe et al. The TG⁻, G⁻G⁺ and TT conformations are found at energies 2.10, 2.85 and 4.75 kcal/mol, respectively, above TG⁻. The relative energy of 2.10 kcal/mol for TG⁻ is in excellent agreement with those of Abe (2.5 kcal/mol).

1,1,1-Trimethoxyethane

The stable conformations found for 1,1,1-trimethoxyethane appear to mirror those found for trimethoxymethane. They are shown in Figure 4. The TTG⁻ conformation is also found to be the most stable, as was found with trimethoxymethane. The relative energies of the TTT, CCC, G⁻TG⁺ and G⁺TG⁺ conformations are 2.41, 4.78, 1.13 and 7.14 kcal/mol. These higher relative energies for TTT, G⁻TG⁺ and G⁺TG⁺, relative to those for the same conformations of trimethoxymethane (0.42, 0.68 and 4.13 kcal/mol), can be explained by the increased steric crowding from additional methyl group here. However, we have yet to explain the stabilization

observed for the CCC conformation (8.72 kcal/mol for trimethoxymethane vs. 4.78 kcal for 1,1,1-trimethoxyethane).

2,2-Dimethoxypropane

Figure 5 shows the stable conformations found for 2,2-dimethoxypropane. The stable conformations appear to mirror, again, those found for dimethoxymethane, with slight variation. The TG⁻, TT, G⁺G⁺ conformations for dimethoxymethane are also found here. However, the G⁻G⁺ is replaced by the A⁺G⁻ conformation. The G⁺G⁺ conformation is again found to be the most stable, with TG⁻, A⁺G⁻ and TT at relative energies of 3.13, 4.45 and 7.01 kcal/mol, respectively.

For 1,1-Dimethoxyethane, the two hydrogen atoms attached to the central carbon of dimethoxymethane are each replaced by methyl groups. Hence, we expect to find larger relative energies for the conformations. The G⁺G⁺ conformation is found to be the most stable.

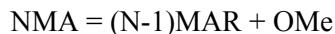
1,1-Dimethoxyethane

The six stable conformations found for 1,1-dimethoxyethane are shown in Figure 6. The G⁺G⁺G⁻ conformer is found to be the most stable, with TT, TG⁺G⁺, TG⁺G⁺, G⁺A⁺G⁻ and G⁻G⁺T at relative energies of 4.66, 3.50, 0.51, 6.48 and 1.09 kcal/mol, respectively. There appears to be some controversy in 1,1-dimethoxyethane. Goodman and Niu have suggested that TG⁺G⁺ is the most stable, while Saur suggests the G⁻G⁺T conformation to be the most stable.

Enthalpies of Formation.

The CBS-Q standard enthalpies appear to agree very well with the experimental data. The worst agreement is for tetramethoxymethane (4MM), deviating by about 1.5 kcal/mol. However, the remaining enthalpies for stable species appear to agree to within about 1 kcal/mol. Interestingly, the B3LYP/6-31G(d,p) enthalpies agree extremely well, with maximum deviation of around 0.75 kcal/mol. However we believe that this is simply a fortuitous coincidence. Examination of enthalpy calculations for several *different* isodesmic reactions reveals the “tightness” or precision of enthalpy data using the CBS-Q method. By calculating the enthalpy of formation for tetramethoxymethane (4MM) using four different isodesmic reactions, we have found the CBS-Q method to give a mean average deviation of 0.365 kcal/mol from the arithmetic average, versus 0.525 and 0.745 for the B3LYP/6-31G(d,p) and B3LYP/6-311+G(3df,2p) methods, respectively.

Table VII gives trends in the bond dissociation energies (BDEs) of the bond connecting oxygen to the central carbon. The BDE is defined here as the enthalpy of reaction for the following reaction.



What is clear from the Table VII is the increasing bond energy with increasing methoxy substitution, due to the anomeric stabilization effect. There is a small increase in BDE with increasing methyl substitution, for the ethers. The steric crowding due to the addition of the third methyl group is the most likely explanation for the calculated BDE decrease. A similar phenomena is also observed for the dimethoxy-substituted species, with the bond stabilizing after the substitution of one hydrogen with a methyl group, followed by bond destabilization after the

substitution with the second methyl group. However for the two trimethoxy-substituted species, the substitution with a methyl group has a dramatic destabilizing effect on the bond, likely due to the steric crowding posed by the three floppy methoxy groups.

Energy Landscapes

Three-dimensional energy landscapes were produced to aid in the visual understanding of the location of the different conformers, as well as the configurational pathways traversed through the course of methoxy rotor motions. For the dimethoxymethane molecule (2MM), the total energy (B3LYP/6-31G(d,p) level) was calculated in the two-dimensional phase space with each of the axes along one of the dihedral angles of each methoxy group. Figure 13 shows the energy landscape of dimethoxymethane. The most clearly recognizable feature in this figure are the large peaks, which represent the CC (eclipsed-eclipsed) conformation of the methoxy groups with respect to each other. In other words, the energy of this conformation is about 20 kcal/mol. However, the most significant barriers to rotation appear to be the “walls” whose corners are marked by the CC peaks. These are the all XC conformations, or X-eclipsed, where X appears to be any local conformation.

Conclusions

In this manuscript, we report, to our knowledge, the first complete thermochemical data for a family of polymethoxyalkane species. The data will not only facilitate modeling studies of the combustion and degradation of these potential fuel additives, but also provide the basis for determination of Benson groups, which may then be used to calculate thermochemistry for other much larger compounds. We have examined the effect of methyl and methoxy substitution on bond energies, and have found that anomeric stabilization due to increased methoxy substitution is eventually offset by destabilization due to steric crowding of the methoxy and methyl groups. This suggests that the breaking of the C-O bond is facilitated in either species with fewer methoxy groups attached to the central carbon, such as methanol (less anomeric stabilization) or in species such as 1,1,1-trimethoxyethane, in which steric crowding plays a strong role in bond destabilization.

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Tables.

Table I. List of Species Examined for $C_cG_1G_2G_3G_4$, where C_c refers to the central carbon, and G_i are the attached groups. The short-hand notation for each species given in parentheses, in Column 5, will be used throughout this report. See text for explanation.

G_1	G_2	G_3	G_4	Species
OMe	OMe	OMe	OMe	Tetramethoxymethane (4MM)
OMe	OMe	OMe	H	Trimethoxymethane (3MM)
OMe	OMe	OMe	Me	1,1,1-Trimethoxyethane (3ME)
OMe	OMe	OMe	DB	Trimethoxymethyl Radical (3MMR)
OMe	OMe	H	H	Dimethoxymethane (2MM)
OMe	OMe	Me	H	1,1-Dimethoxyethane (2ME)
OMe	OMe	Me	Me	2,2-Dimethoxypropane (2MP)
OMe	OMe	H	DB	Dimethoxymethyl Radical (2MMR)
OMe	OMe	Me	DB	1,1-Dimethoxyethyl Radical (2MER)
OMe	H	H	DB	Methoxymethyl Radical (MMR)
OMe	Me	H	DB	1-Methoxy 1-Ethyl Radical (MER)
OMe	Me	Me	DB	2-Methoxy 2-Propyl Radical (MPR)

Table II: Isodesmic reactions used in this study. The convention goes as follows: A + B = C + D, where A is the species of interest, and species B, C and D are either the known isodesmic species listed in Appendix A, or are species whose standard heat of formation has been calculated previously in this report. All reactions are isodesmic, with the exception of those marked in column 5, which are group-conserving, in addition to being isodesmic.

A	B	C	D	IG
Tetramethoxymethane	Ethane	Trimethoxymethane	Methyl Ethyl Ether	
Trimethoxymethane	Ethane	Dimethoxyethane	Methyl Ethyl Ether	
Dimethoxymethane	Ethane	Dimethyl Ether	Methyl Ethyl Ether	
1,1,1-Trimethoxymethane	t-Butanol	2,2-dihydroxypropane	2,2-dihydroxypropane	
2,2-Dimethoxypropane	Neopentane	t-Butanol	t-Butanol	
1,1-Dimethoxyethane	Isobutane	Isopropanol	Isopropanol	
Trimethoxymethyl radical	Trihydroxymethane	Trihydroxymethyl Radical	Trimethoxymethane	X
Dimethoxymethyl radical	Dihydroxymethane	Dihydroxymethyl Radical	Dimethoxymethane	X
Methoxymethyl radical	Methanol	Dimethyl Ether	Methanol Radical	
1,1-Methoxyethane 1-yl radical	Isobutane	t-Butyl Radical	1,1-dihydroxyethane	
2-Methoxy 2-yl radical	Isobutane	t-Butyl Radical	Isopropanol	
1-Methoxy 1-yl radical	Propane	Isopropyl Radical	Ethanol	

Table III: The standard heat of formations are shown here for twelve species, at the B3LYP/6-31G(d,p) level (B3LYP, Column 2), the B3LYP/6-311+G(3df,2p)//B3LYP/6-31G(d,p) level (B3LYP+, Column 3) and the CBS-Q level (Column 4). Uncertainties for columns two and three are the same as for those listed in Column 5. Column 6 shows the available experimental values for ΔH_f^0 .

Species	ΔH_f^0 (B3LYP)	ΔH_f^0 (B3LYP+)	ΔH_f^0 (CBS-Q)	ΔH_f^0 (expt)
Tetramethoxymethane	-173.80	-170.88	-175.27 ± 0.81	-173.80 ± 0.30
Trimethoxymethane	-126.63	-125.17	-127.49 ± 0.58	-127.10 ± 0.77
Dimethoxymethane	-83.89	-82.89	-83.97 ± 0.35	-83.21 ± 0.19
1,1,1-Trimethoxymethane	-136.33	-135.80	-135.50 ± 1.83	-136.44 ± 0.21
2,2-Dimethoxypropane	-102.12	-101.26	-102.52 ± 0.76	-101.5 ± 0.30
1,1-Dimethoxyethane	-93.10	-92.54	-93.86 ± 0.61	-93.15 ± 0.20
Trimethoxymethyl radical	-84.87	-86.02	-84.97 ± 2.59	
Dimethoxymethyl radical	-37.65	-38.68	-38.06 ± 1.45	
Methoxymethyl radical	0.25	-0.36	-0.25 ± 0.79	
1,1-Dimethoxyethyl radical	-51.24	-52.25	-51.89 ± 1.46	
2-Methoxyp propane 2-yl radical	-18.64	-19.09	-19.53 ± 1.08	
1-Methoxyethane 1-yl radical	-8.35	-8.37	-8.34 ± 0.78	

Table IV: B3LYP/6-31G(d,p) Unscaled vibrational frequencies (cm-1) of each conformation (Column 2) of each species (Column 1). (See text for explanation on the notation)

Species	Conf.	Frequencies
4MM	TTTT	95 99 110 111 152 153 177 177 196 296 296 329 454 467 589 589 671 760 1048 1062 1062 1127 1146 1146 1158 1182 1182 1182 1193 1222 1224 1236 1236 1473 1478 1489 1489 1499 1500 1500 1502 1524 1524 1528 1529 3047 3047 3047 3048 3121 3121 3122 3123 3146 3146 3146 3146
	G ⁻ G ⁺ G ⁻ G ⁺	64 101 101 108 168 168 172 180 211 269 337 337 441 471 500 661 661 781 1021 1021 1097 1124 1151 1167 1167 1184 1190 1190 1190 1213 1213 1227 1239 1477 1481 1481 1495 1495 1499 1499 1499 1516 1529 1529 1544 3044 3044 3045 3046 3109 3111 3111 3111 3112 3151 3151 3151 3151
	A ⁺ G ⁺ G ⁻ G ⁺	47 54 92 104 146 162 172 205 213 254 326 347 420 467 550 609 655 756 1032 1052 1072 1112 1144 1167 1174 1178 1184 1185 1193 1214 1217 1222 1246 1473 1477 1486 1490 1494 1495 1501 1504 1520 1526 1529 1535 3030 3032 3046 3048 3101 3102 3116 3119 3141 3148 3149 3150
3MM	TTG ⁻	100 111 115 153 169 181 264 304 342 503 558 691 954 1006 1042 1110 1145 1163 1180 1184 1188 1215 1223 1252 1387 1408 1475 1490 1492 1498 1500 1502 1524 1527 1529 2964 3005 3009 3048
	TTT	102 104 109 163 174 175 293 294 319 543 544 607 1035 1039 1040 1143 1143 1144 1181 1185 1185 1227 1227 1257 1402 1406 1481 1493 1494 1498 1500 1500 1525 1528 1528 2848 3002 3002 3005
	CCC	90 91 115 170 175 204 306 308 319 520 521 720 928 962 963 1122 1122 1174 1180 1181 1191 1215 1215 1221 1407 1407 1473 1483 1484 1504 1505 1520 1521 1533 1533 3015 3016 3026 3088 3103 3103 3105 3145 3145 3145
	G ⁻ TG ⁺	77 99 105 152 162 207 231 302 359 482 566 702 933 1015 1057 1107 1148 1161 1178 1184 1185 1212 1213 1259 1396 1408 1473 1489 1495 1497 1500 1500 1521 1526 1533 2971 3008 3010 3043 3077 3078 3110 3146 3147 3148
	G ⁺ TG ⁺	63 100 125 145 189 210 222 331 358 475 554 599 979 1017 1072 1113 1164 1170 1180 1182 1184 1212 1219 1278 1390 1423 1485 1490 1495 1497 1502 1507 1522 1528 1531 2883 2995 2995 3007 3061 3077 3078 3138 3146 3147
2MM	TG ⁻	81 130 169 231 325 384 559 971 993 1125 1139 1177 1183 1203 1231 1248 1308 1444 1482 1495 1500 1504 1521 1527 1542 2898 2980 3002 3019 3025 3089 3135 3144
	TT	79 83 218 220 233 426 479 1011 1047 1153 1170 1171 1181 1203 1225 1255 1274 1453 1488 1500 1500 1504 1519 1533 1567 2874 2890 2981 2983 3027 3028 3141 3141
	G ⁺ G ⁺	104 129 146 219 320 454 604 940 955 1077 1146 1165 1181 1182 1216 1258 1340 1434 1476 1495 1496 1499 1513 1522 1530 2998 3002 3009 3058 3075 3077 3139 3140
	G ⁻ G ⁺	-11 132 149 229 380 438 562 924 956 1096 1107 1177 1179 1210 1213 1255 1350 1447 1480 1490 1504 1505 1516 1517 1531 2941 2993 3002 3055 3066 3120 3121 3124

Species	Conf.	Frequencies
3ME	TTT	64 81 84 155 171 174 258 258 267 356 391 392 541 565 566 736 920 922 1091 1091 1117 1160 1181 1182 1183 1188 1188 1242 1243 1249 1411 1476 1482 1482 1497 1498 1509 1517 1518 1525 1528 1529 3018 3018 3020 3072 3099 3099 3099 3141 3141 3141 3150 3151
	TTG ⁻	67 101 115 155 169 187 216 254 297 320 386 407 524 566 622 741 902 913 1074 1094 1109 1160 1177 1182 1183 1186 1203 1221 1242 1267 1418 1472 1481 1483 1495 1498 1503 1507 1518 1525 1528 1531 3019 3025 3048 3076 3087 3104 3122 3133 3142 3145 3155 3162
	G ⁻ TG ⁺	66 96 117 174 192 213 233 284 325 336 370 423 501 539 593 724 907 910 1084 1105 1131 1163 1176 1179 1182 1186 1208 1221 1229 1270 1417 1479 1480 1486 1496 1504 1505 1512 1520 1526 1529 1531 3001 3011 3018 3071 3076 3080 3088 3130 3138 3140 3142 3162
	CCC	78 83 101 158 171 201 258 282 283 330 377 378 534 534 625 726 895 896 1092 1105 1105 1160 1161 1174 1182 1183 1216 1218 1219 1267 1425 1473 1480 1480 1497 1497 1503 1504 1519 1522 1533 1533 3013 3014 3025 3073 3100 3100 3102 3141 3141 3141 3160 3160
	G ⁺ TG ⁺	60 119 127 159 181 185 235 258 292 350 390 401 485 604 615 751 900 912 1070 1071 1146 1150 1180 1183 1184 1194 1210 1221 1226 1274 1424 1472 1481 1486 1493 1497 1502 1513 1517 1528 1530 1537 3020 3022 3044 3077 3085 3087 3112 3135 3136 3144 3157 3161
	2MP	78 85 190 202 230 280 302 355 356 369 472 489 528 732 853 906 971 1001 1096 1162 1183 1184 1194 1214 1223 1243 1271 1407 1422 1485 1491 1494 1494 1505 1507 1523 1525 1527 1531 3000 3001 3051 3054 3061 3063 3125 3126 3127 3133 3144 3146
2ME	TG ⁻	91 95 173 191 233 267 279 314 363 382 459 502 563 728 854 919 952 1006 1106 1122 1179 1184 1196 1200 1214 1261 1274 1408 1422 1475 1488 1491 1496 1503 1509 1516 1524 1529 1529 3002 3016 3052 3062 3066 3096 3122 3134 3137 3139 3143 3154
	A ⁺ G ⁻	100 126 196 229 238 268 292 308 358 386 437 505 575 724 836 932 943 1015 1109 1126 1176 1179 1188 1200 1219 1245 1289 1414 1427 1480 1489 1492 1496 1504 1506 1516 1523 1528 1532 2997 3013 3063 3067 3068 3073 3124 3127 3137 3144 3148 3154
	G ⁺ G ⁺	121 134 165 190 212 261 262 306 352 393 418 553 583 737 837 931 945 1012 1089 1116 1176 1185 1185 1208 1221 1246 1292 1413 1425 1475 1484 1491 1492 1503 1508 1514 1522 1528 1532 3017 3018 3063 3068 3084 3086 3129 3129 3140 3146 3148 3149
	TTG ⁺	49 62 182 204 239 252 347 444 467 534 848 916 1071 1088 1135 1164 1171 1183 1187 1216 1263 1387 1404 1422 1487 1488 1496 1501 1506 1518 1526 1527 2905 2985 2987 3034 3035 3055 3122 3132 3132 3145
3MMR	TG ⁻ G ⁺	37 87 172 192 225 272 362 398 463 617 829 903 1013 1082 1123 1139 1177 1184 1189 1230 1247 1383 1408 1422 1481 1488 1497 1501 1510 1515 1526 1526 2986 3006 3018 3035 3058 3094 3127 3129 3138 3143
	TG ⁺ G ⁺	82 123 172 192 224 276 328 402 529 553 844 907 1054 1104 1127 1148 1173 1180 1185 1221 1254 1390 1404 1431 1482 1487 1496 1497 1505 1510 1525 1528 2905 2986 2999 3035 3062 3087 3128 3137 3142 3149
	G ⁺ A ⁺ G ⁻	106 122 193 229 271 284 318 414 477 647 798 875 1006 1048 1119 1143 1174 1180 1203 1221 1234 1389 1418 1423 1479 1490 1501 1505 1510 1519 1524 1531 3001 3015 3062 3069 3073 3073 3127 3129 3136 3146
	G ⁺ G ⁺ G ⁻	105 125 155 193 248 287 302 392 534 637 822 886 1016 1077 1119 1151 1173 1180 1183 1220 1237 1386 1409 1430 1475 1486 1497 1498 1504 1518 1524 1530 3002 3012 3019 3065 3077 3084 3132 3138 3144 3147
2MMR	G ⁺ G ⁺ T	-56 111 137 216 229 267 346 392 532 564 844 887 1048 1106 1123 1128 1178 1179 1186 1217 1249 1382 1401 1431 1486 1489 1498 1499 1509 1515 1518 1531 2936 2994 3002 3054 3066 3068 3117 3119 3150 3153
	TTG ⁻	77 86 92 136 151 167 240 278 328 512 567 701 901 977 1053 1122 1152 1155 1178 1180 1195 1209 1235 1272 1467 1486 1490 1497 1498 1501 1518 1520 1526 3035 3040 3044 3105 3114 3122 3149 3152 3157
	G ⁻ TG ⁺	68 83 88 129 131 163 224 271 340 485 580 716 893 990 1023 1113 1156 1159 1179 1182 1195 1206 1253 1258 1464 1488 1491 1496 1498 1515 1522 1528 3035 3037 3041 3104 3104 3113 3153 3153 3156
	TTT	77 83 85 140 150 154 262 263 321 547 548 612 950 1053 1054 1146 1175 1175 1178 1194 1194 1243 1255 1256 1478 1488 1488 1497 1499 1499 1523 1523 3031 3031 3034 3107 3107 3107 3149 3150 3150
2MMR	A ⁺ A ⁺ G ⁺	69 93 102 123 172 190 219 316 320 481 564 612 918 1030 1073 1131 1175 1175 1175 1181 1181 1209 1211 1265 1282 1483 1487 1490 1497 1502 1505 1518 1524 1528 3022 3022 3028 3090 3096 3097 3139 3152 3152
	TG ⁻	55 97 160 172 295 360 580 876 947 1035 1156 1161 1178 1186 1239 1264 1362 1479 1497 1500 1500

Species	Conf.	Frequencies
		1517 1518 2998 3014 3022 3076 3103 3150 3152
	TT	79 105 189 190 216 429 494 964 1029 1066 1178 1180 1187 1188 1253 1309 1377 1490 1499 1500 1504 1518 1520 2932 3004 3008 3067 3067 3150 3150
	TG ⁺	87 115 169 200 288 372 586 937 967 1042 1157 1173 1181 1206 1241 1284 1374 1484 1495 1499 1502 1518 1521 3008 3033 3065 3070 3109 3146 3151
	A'G ⁻	37 105 158 188 311 417 603 873 945 986 1129 1164 1174 1189 1217 1240 1380 1477 1494 1498 1500 1513 1522 3016 3036 3083 3108 3117 3141 3153
MMR		172 300 430 652 974 1144 1175 1258 1298 1469 1499 1511 1516 3010 3072 3108 3147 3261
2MER	G ⁺ G ⁺	66 97 153 165 187 267 290 407 497 559 801 937 1074 1085 1101 1173 1179 1195 1210 1260 1315 1418 1481 1484 1489 1497 1502 1509 1521 1523 2993 3015 3031 3074 3101 3108 3137 3145 3148
	TG ⁺	39 71 152 174 227 245 337 440 481 493 800 947 1064 1074 1135 1176 1177 1190 1214 1287 1317 1418 1485 1486 1492 1497 1510 1513 1521 1524 2979 3010 3014 3070 3071 3103 3137 3139 3140
	G ⁺ G ⁺	69 90 136 154 184 250 269 388 538 603 788 923 994 1067 1083 1159 1177 1182 1202 1250 1277 1418 1472 1483 1486 1497 1499 1509 1515 1524 2981 3025 3035 3092 3097 3104 3144 3146 3148
MPR		107 156 161 216 297 338 376 496 770 951 959 977 1087 1126 1173 1203 1299 1315 1415 1430 1477 1489 1492 1494 1505 1516 1521 2941 2960 3011 3070 3072 3075 3119 3124 3136
MER	C	109 161 199 286 471 607 891 1032 1077 1132 1177 1201 1286 1390 1435 1479 1492 1499 1512 1516 2971 3006 3066 3067 3105 3124 3143
MER	T	146 177 256 307 491 611 874 1008 1029 1128 1172 1213 1296 1391 1435 1484 1490 1499 1511 1520 2953 3014 3056 3074 3118 3140 3188

Table V: Rotational constants (GHz) for each conformer (Column 2) of each Species (Column 1). (See the text for explanation about the notation).

Species	Conformer	I ₁ (GHz)	I ₂ (GHz)	I ₃ (GHz)
4MM	TTTT	1.6718424	1.4518028	1.4516636
	G ⁻ G ⁺ G ⁻ G ⁺	1.8281791	1.8280762	1.1495096
	A ⁺ G ⁺ G ⁻ G ⁺	1.8269963	1.5631405	1.2969372
3MM	TTG ⁻	3.0247593	2.4608924	1.5552144
	TTT	2.6554620	2.6549483	1.4336703
	CCC	2.7775661	2.7770944	1.8948017
	G ⁻ TG ⁺	3.7405892	2.1001570	1.5644421
	G ⁺ TG ⁺	3.4547517	2.2058138	1.4525622
2MM	TG ⁻	14.2065270	2.7840519	2.5500413
	TT	24.3176255	2.3115614	2.1997417
	G ⁺ G ⁺	10.3447591	3.2162796	3.0268469
	G ⁻ G ⁺	9.1571031	3.5422296	2.8131681
3ME	TTT	2.0965092	2.0949985	1.3876917
	TTG ⁻	2.2442189	1.9205931	1.5283675
	G ⁻ TG ⁺	2.5642872	1.7900037	1.4117795
	CCC	1.9444997	1.9431594	1.8838684
	G ⁺ TG ⁺	2.6826850	1.8004859	1.4359884
2MP	TT	4.2940035	1.7787396	1.7785734
	TG ⁻	3.3147768	2.1573002	1.8737119
	A ⁺ G ⁻	2.7402975	2.6036307	1.9340395
	G ⁺ G ⁺	2.9150415	2.4871831	1.9546294
ME	TTG ⁺	6.5224740	2.2261591	1.8583954
	TG ⁻ G ⁺	5.5720774	2.5236663	2.0563983
	TG ⁺ G ⁺	4.7273157	2.8582506	1.9468362
	G ⁺ A ⁻ G ⁻	4.5151321	2.9914563	2.3851658
	G ⁺ G ⁺ G ⁻	4.4806288	3.0788344	2.1913164
	G ⁻ G ⁺ T	3.7872867	3.4911196	1.9748555
3MMR	TTG ⁻	3.0472737	2.5004071	1.5409388
	G ⁻ TG ⁺	3.8032850	2.1204767	1.5577491
	TTT	2.7005934	2.6919539	1.4336841
	A ⁺ A ⁺ G ⁺	3.5907814	2.2171183	1.4595856
2MMR	TG ⁻	15.8158876	2.7851093	2.5651286
	TT	27.0358096	2.3352136	2.2180210
	TG ⁺	15.2973693	2.8800998	2.5611294
	A ⁻ G ⁻	11.9762916	3.1275954	2.8739879
MMR		47.1974820	10.6380935	9.2411154
2MER	G ⁺ G ⁺	4.9787643	2.8809624	1.9405350
	TG ⁺	7.3050018	2.2341083	1.8383839
	G ⁺ G ⁺	4.4030596	3.2302057	2.1568522
MPR		7.7945990	3.9285627	2.7748287
MER	C	34.1612216	4.1457487	3.8885871
	T	16.0565831	5.7361598	4.5278321

Table VI: Summary of thermodynamic data S^0_{298} and C_p . Listed are the standard enthalpy of formation and heat capacities at different temperatures, for each conformation (Column 2) of each Species (Column 1). (See text for explanation of the notation). For each conformation, the translational, vibrational and rotational (TVR), the internal rotation (IR) and total components of S^0_{298} and C_p are listed. For rows in Column 3 listed as “Equil,” the values of S^0_{298} and C_p for the gas-phase species with an equilibrium mixture of all conformations are given.

Spec	Conf		S^0_{298}	C_p300	C_p400	C_p500	C_p600	C_p800	C_p1000	C_p1500
4MM	TTT	TVR	51.452	25.791	35.078	43.939	51.662	63.836	72.767	86.450
		IR	40.159	13.071	13.590	13.998	14.363	14.866	14.792	12.595
		Total	91.611	38.862	48.668	57.937	66.025	78.702	87.559	99.045
	$G^+G^+GG^+$	TVR	65.899	25.786	35.069	43.928	51.652	63.834	72.770	86.459
		IR	46.579	16.814	18.400	18.037	16.753	13.651	10.918	6.407
		Total	112.478	42.600	53.469	61.965	68.405	77.485	83.688	92.866
	$A^+G^+G^-G^+$	TVR	66.099	25.920	35.188	44.030	51.740	63.903	72.829	86.498
		IR	36.125	15.360	16.042	16.314	16.289	15.678	14.688	11.966
		Total	102.224	41.280	51.230	60.344	68.029	79.581	87.517	98.464
	Equil		102.104	39.005	49.187	58.373	66.984	80.021	89.442	97.964
3MM	TTG ⁻	TVR	65.421	20.275	27.587	34.746	41.067	51.126	58.540	69.891
		IR	32.410	12.292	12.004	11.670	11.279	10.278	9.120	6.582
		Total	97.831	32.567	39.591	46.416	52.346	61.404	67.660	76.473
	TTT	TVR	65.555	20.246	27.497	34.644	40.982	51.097	58.553	69.938
		IR	33.916	15.364	14.462	13.530	12.539	10.441	8.499	5.114
		Total	99.471	35.610	41.959	48.174	53.521	61.538	67.052	75.052
	CCC	TVR	65.102	20.409	27.766	34.912	41.200	51.191	58.559	69.870
		IR	30.429	15.600	14.500	12.704	11.044	8.702	7.359	5.900
		Total	95.531	36.009	42.266	47.616	52.244	59.893	65.918	75.770
	G ⁻ TG ⁺	TVR	65.562	20.316	27.611	34.762	41.080	51.136	58.549	69.899
		IR	31.370	11.195	11.066	10.905	10.661	9.880	8.900	6.759
		Total	96.932	31.511	38.677	45.667	51.741	61.016	67.449	76.658
	G ⁺ TG ⁺	TVR	65.742	20.407	27.628	34.743	41.058	51.148	58.593	69.963
		IR	30.223	13.686	13.564	13.294	12.861	11.583	10.118	7.083
		Total	95.965	34.093	41.192	48.037	53.919	62.731	68.711	77.046
	Equil		97.146	34.012	39.077	47.722	51.838	62.789	67.232	77.727
2MM	TG ⁻	TVR	62.186	15.350	20.635	25.999	30.830	38.643	44.461	53.392
		IR	20.053	8.299	8.954	8.895	8.359	6.950	5.778	4.093
		Total	82.239	23.649	29.589	34.894	39.189	45.593	50.239	57.485
	TT	TVR	62.545	15.461	20.624	25.947	30.779	38.637	44.493	53.454
		IR	18.324	9.103	9.534	9.384	8.894	7.663	6.593	4.881
		Total	80.869	24.564	30.158	35.331	39.673	46.300	51.086	58.335
	G ⁺ G ⁺	TVR	61.936	15.258	20.657	26.061	30.890	38.660	44.439	53.340
		IR	19.307	7.982	9.206	9.379	8.871	7.380	6.150	4.399
		Total	81.243	23.240	29.863	35.440	39.761	46.040	50.589	57.739
	G ⁻ G ⁺	TVR	61.892	15.261	20.658	26.056	30.885	38.665	44.455	53.363
		IR	19.299	7.982	9.206	9.379	8.871	7.380	6.150	4.399
		Total	81.191	23.243	29.864	35.435	39.756	46.045	50.605	57.762
	Equil		81.386	23.692	31.486	36.413	41.413	46.615	51.655	57.679
3ME	TTT	TVR	66.921	24.830	33.621	41.998	49.326	60.964	69.578	82.880
		IR	36.065	14.693	15.169	15.223	14.791	13.292	11.759	8.718
		Total	102.986	39.523	48.790	57.221	64.117	74.256	81.337	91.598
	TTG ⁻	TVR	66.772	24.795	33.615	42.005	49.335	60.963	69.567	82.861
		IR	36.936	14.078	14.205	14.110	13.753	12.530	11.119	8.175
		Total	103.708	38.873	47.820	56.115	63.088	73.493	80.686	91.036
	G ⁻ TG ⁺	TVR	66.540	24.817	33.625	42.005	49.336	60.987	69.611	82.916
		IR	36.295	13.881	14.606	15.071	15.022	13.911	12.328	8.697
		Total	102.835	38.698	48.231	57.076	64.358	74.898	81.939	91.613

Spec	Conf		S^0_{298}	C _p 300	C _p 400	C _p 500	C _p 600	C _p 800	C _p 1000	C _p 1500
	CCC	TVR	66.764	24.940	33.742	42.111	49.423	61.031	69.622	82.898
		IR	30.714	16.238	15.988	15.220	14.308	12.636	11.367	9.344
		Total	97.478	41.178	49.730	57.331	63.731	73.667	80.989	92.242
	G ⁺ TG ⁺	TVR	66.614	24.739	33.561	41.954	49.290	60.935	69.552	82.861
		IR	39.812	13.636	13.254	12.868	12.513	11.697	10.636	7.748
		Total	106.426	38.375	46.815	54.822	61.803	72.632	80.188	90.609
		Equil	102.686	39.647	48.929	56.815	64.028	74.156	81.760	91.619
2MP	TT	TVR	65.361	23.665	32.001	39.932	46.894	58.032	66.350	79.294
		IR	31.662	12.430	12.359	12.043	11.575	10.454	9.350	7.129
		Total	97.023	36.095	44.360	51.975	58.469	68.486	75.700	86.423
	TG ⁻	TVR	65.562	23.707	32.048	39.980	46.933	58.048	66.346	79.273
		IR	34.301	10.755	11.372	11.672	11.485	10.230	8.765	6.067
		Total	99.863	34.462	43.420	51.652	58.418	68.278	75.111	85.340
	A ⁺ G ⁻	TVR	65.540	23.730	32.062	39.986	46.935	58.048	66.347	79.274
		IR	27.644	13.493	14.777	15.364	15.059	13.003	10.768	7.182
		Total	93.184	37.223	46.839	55.350	61.994	71.051	77.115	86.456
	G ⁺ G ⁺	TVR	65.646	23.703	32.045	39.979	46.931	58.038	66.330	79.253
		IR	31.831	11.576	13.089	13.925	13.831	12.061	9.963	6.398
		Total	97.477	35.279	45.134	53.904	60.762	70.099	76.293	85.651
		Equil	96.887	35.418	46.271	55.051	62.470	71.042	77.260	85.977
2ME	TTG ⁺	TVR	65.742	20.407	27.628	34.743	41.058	51.148	58.593	69.963
		IR	32.647	12.536	12.046	11.375	10.648	9.226	8.017	5.976
		Total	98.389	32.943	39.674	46.118	51.706	60.374	66.610	75.939
	TG ⁻ G ⁺	TVR	66.241	19.349	26.189	32.870	38.789	48.284	55.358	66.306
		IR	24.570	9.959	10.763	11.195	11.174	10.255	8.958	6.285
		Total	90.811	29.308	36.952	44.065	49.963	58.539	64.316	72.591
	TG ⁺ G ⁺	TVR	66.377	19.308	26.122	32.806	38.740	48.270	55.368	66.333
		IR	27.055	11.289	10.967	10.505	9.880	8.424	7.110	4.923
		Total	93.432	30.597	37.089	43.311	48.620	56.694	62.478	71.256
	G ⁺ A ⁺ G ⁻	TVR	66.176	19.414	26.270	32.941	38.840	48.298	55.348	66.280
		IR	23.047	10.599	10.981	11.286	11.352	10.706	9.483	6.610
		Total	89.223	30.013	37.251	44.227	50.192	59.004	64.831	72.890
	G ⁺ G ⁺ G ⁻	TVR	66.234	19.307	26.173	32.868	38.787	48.271	55.335	66.277
		IR	27.692	8.981	8.824	8.699	8.524	7.884	7.025	5.153
		Total	93.926	28.288	34.997	41.567	47.311	56.155	62.360	71.430
	G ⁻ G ⁺ T	TVR	66.373	19.325	26.159	32.846	38.774	48.289	55.377	66.332
		IR	28.967	10.299	9.177	8.208	7.436	6.288	5.493	4.349
		Total	95.340	29.624	35.336	41.054	46.210	54.577	60.870	70.681
		Equil	92.269	29.761	35.593	43.209	47.842	57.447	62.400	72.501
3MMR	TTG ⁻	TVR	67.087	20.186	27.021	33.607	39.365	48.459	55.136	65.372
		IR	34.990	11.839	11.200	10.550	9.988	8.997	8.023	5.813
		Total	102.077	32.025	38.221	44.157	49.353	57.456	63.159	71.185
	G ⁺ TG ⁺	TVR	67.166	20.230	27.057	33.638	39.392	48.481	55.156	65.387
		IR	33.507	11.883	11.357	10.507	9.693	8.374	7.373	5.726
		Total	100.673	32.113	38.414	44.145	49.085	56.855	62.529	71.113
	TTT	TVR	67.187	20.096	26.836	33.397	39.166	48.312	55.035	65.330
		IR	32.575	14.135	12.403	10.993	9.973	8.631	7.723	6.179
		Total	99.762	34.231	39.239	44.390	49.139	56.943	62.758	71.509
	A ⁺ A ⁺ G ⁺	TVR	67.234	20.233	26.954	33.491	39.244	48.373	55.089	65.371
		IR	35.919	12.075	10.488	9.275	8.380	7.146	6.300	4.964
		Total	103.153	32.308	37.442	42.766	47.624	55.519	61.389	70.335
		Equil	101.416	34.654	41.725	45.643	51.693	57.716	64.386	70.874
2MMR	TG ⁻	TVR	63.691	15.491	20.393	25.199	29.442	36.209	41.223	48.949
		IR	22.416	8.250	7.715	6.951	6.279	5.291	4.619	3.608
		Total	86.107	23.741	28.108	32.150	35.721	41.500	45.842	52.557
	TT	TVR	63.853	15.347	20.106	24.886	29.156	36.015	41.103	48.916
		IR	26.431	9.902	8.803	7.359	6.133	4.404	3.300	1.825

Spec	Conf		S ⁰ ₂₉₈	C _p 300	C _p 400	C _p 500	C _p 600	C _p 800	C _p 1000	C _p 1500
		Total	90.284	25.249	28.909	32.245	35.289	40.419	44.403	50.741
	TG ⁺	TVR	63.619	15.308	20.175	24.986	29.248	36.053	41.096	48.870
		IR	21.500	9.774	8.804	7.696	6.799	5.567	4.777	3.655
		Total	85.119	25.082	28.979	32.682	36.047	41.620	45.873	52.525
	A ⁻ G ⁻	TVR	63.422	15.391	20.391	25.233	29.478	36.219	41.207	48.912
		IR	22.242	7.274	7.027	6.641	6.254	5.573	5.011	3.995
		Total	85.664	22.665	27.418	31.874	35.732	41.792	46.218	52.907
		Equil	86.794	26.811	30.273	33.531	36.441	41.607	45.584	51.912
MMR		TVR	58.457	11.831	14.705	17.544	20.082	24.226	27.394	32.453
		IR	9.613	2.563	2.656	2.703	2.713	2.663	2.576	2.377
		Total	68.070	14.394	17.361	20.247	22.795	26.889	29.970	34.830
		Equil	68.070	14.394	17.36	20.25	22.795	26.889	29.97	34.83
2MER	G ⁺ G ⁺	TVR	65.746	19.171	25.438	31.525	36.900	45.499	51.893	61.786
		IR	27.599	8.416	8.571	8.408	8.024	7.090	6.302	5.069
		Total	93.345	27.587	34.009	39.933	44.924	52.589	58.195	66.855
	TG ⁺	TVR	65.639	19.183	25.419	31.490	36.865	45.481	51.893	61.804
		IR	32.745	8.018	8.763	8.891	8.439	6.870	5.387	3.073
		Total	98.384	27.201	34.182	40.381	45.304	52.351	57.280	64.877
	G ⁺ G ⁺	TVR	65.855	19.304	25.649	31.755	37.116	45.663	52.012	61.844
		IR	29.361	8.990	9.155	8.850	8.349	7.263	6.300	4.561
		Total	95.216	28.294	34.804	40.605	45.465	52.926	58.312	66.405
		Equil	95.649	28.124	35.695	40.872	46.663	53.325	59.459	66.447
MPR		TVR	63.277	18.083	23.871	29.514	34.530	42.642	48.746	58.269
		IR	23.807	7.195	6.449	5.817	5.315	4.577	4.055	3.250
		Total	87.084	25.278	30.320	35.331	39.845	47.219	52.801	61.519
		Equil	87.084	25.278	30.32	35.33	39.845	47.219	52.8	61.52
MER	T	TVR	62.267	14.641	19.012	23.312	27.141	33.343	38.023	45.356
		IR	13.995	6.091	5.921	5.502	5.072	4.409	3.989	3.477
		Total	76.262	20.732	24.933	28.814	32.213	37.752	42.012	48.833
	C	TVR	62.395	14.637	19.052	23.359	27.181	33.362	38.025	45.343
		IR	14.608	5.282	5.338	5.078	4.755	4.215	3.860	3.417
		Total	77.003	19.919	24.390	28.437	31.936	37.577	41.885	48.760
		Equil	76.633	21.113	26.246	29.321	33.349	37.889	42.747	48.586

Table VII: Trends in bond dissociation energies: oxygen-central carbon bond. BDE is enthalpy of reaction for NMA = (N-1)MAR + OMe (See text for explanation of notation).

Bond	NMA	(N-1)MAR	BDE(kcal/mol)
MeO-C/H/H/H	Dimethyl Ether	Methyl Radical	82.91
MeO-C/Me/H/H	Methyl Ethyl Ether	Ethyl Radical	84.23
MeO-C/Me/Me/H	Methyl Isopropyl Ether	Isopropyl Radical	86.34
MeO-C/Me/Me/Me	Methyl t-Butyl Ether	t-Butyl Radical	82.78
MeO-C/OMe/H/H	2MM	MMR	87.82
MeO-C/OMe/Me/H	2ME	MER	89.62
MeO-C/OMe/Me/Me	2MP	MPR	87.09
MeO-C/OMe/OMe/H	3MM	2MMR	93.53
MeO-C/OMe/OMe/Me	3ME	2MER	87.71
MeO-C/OMe/OMe/OMe	4MM	3MMR	94.40

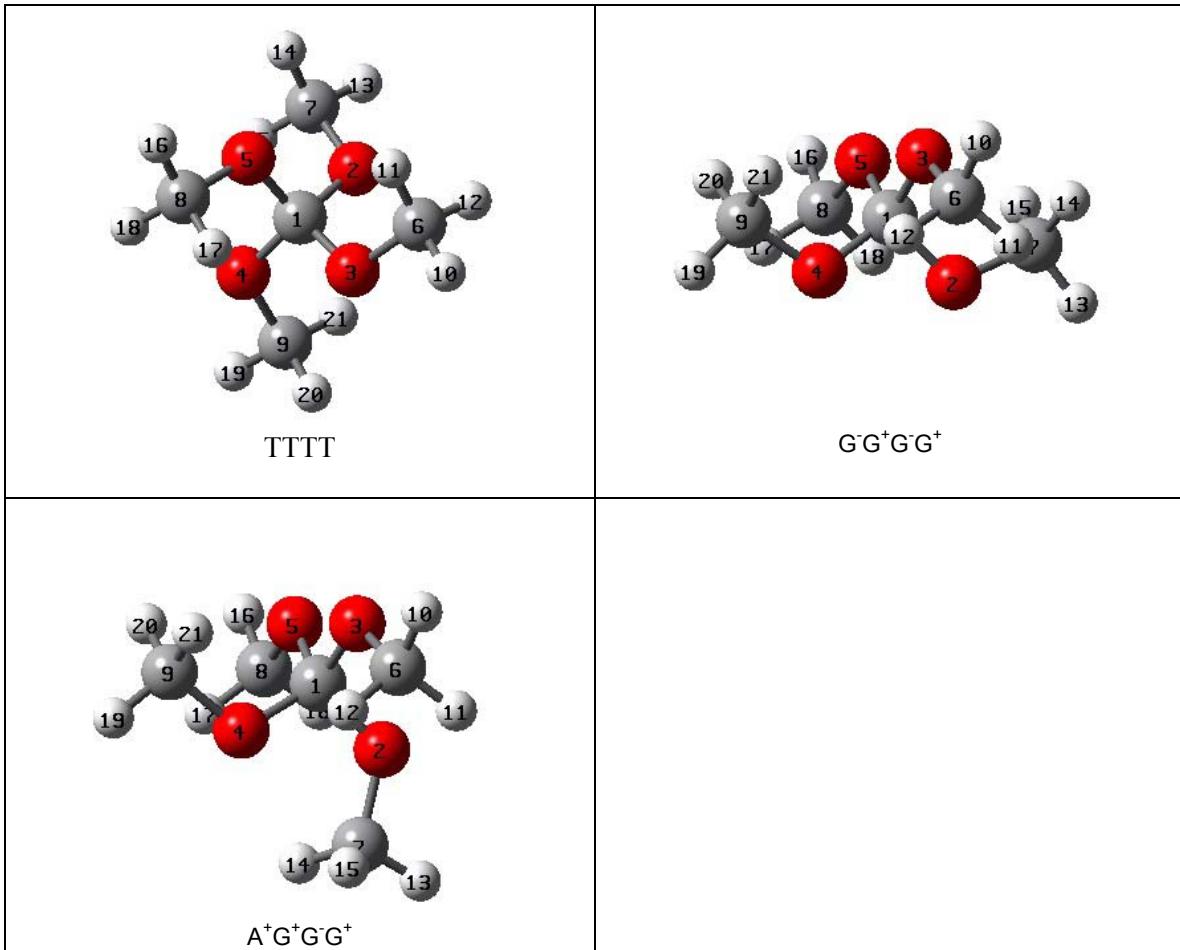


Figure 1: Stable conformations of Tetramethoxymethane (4MM)

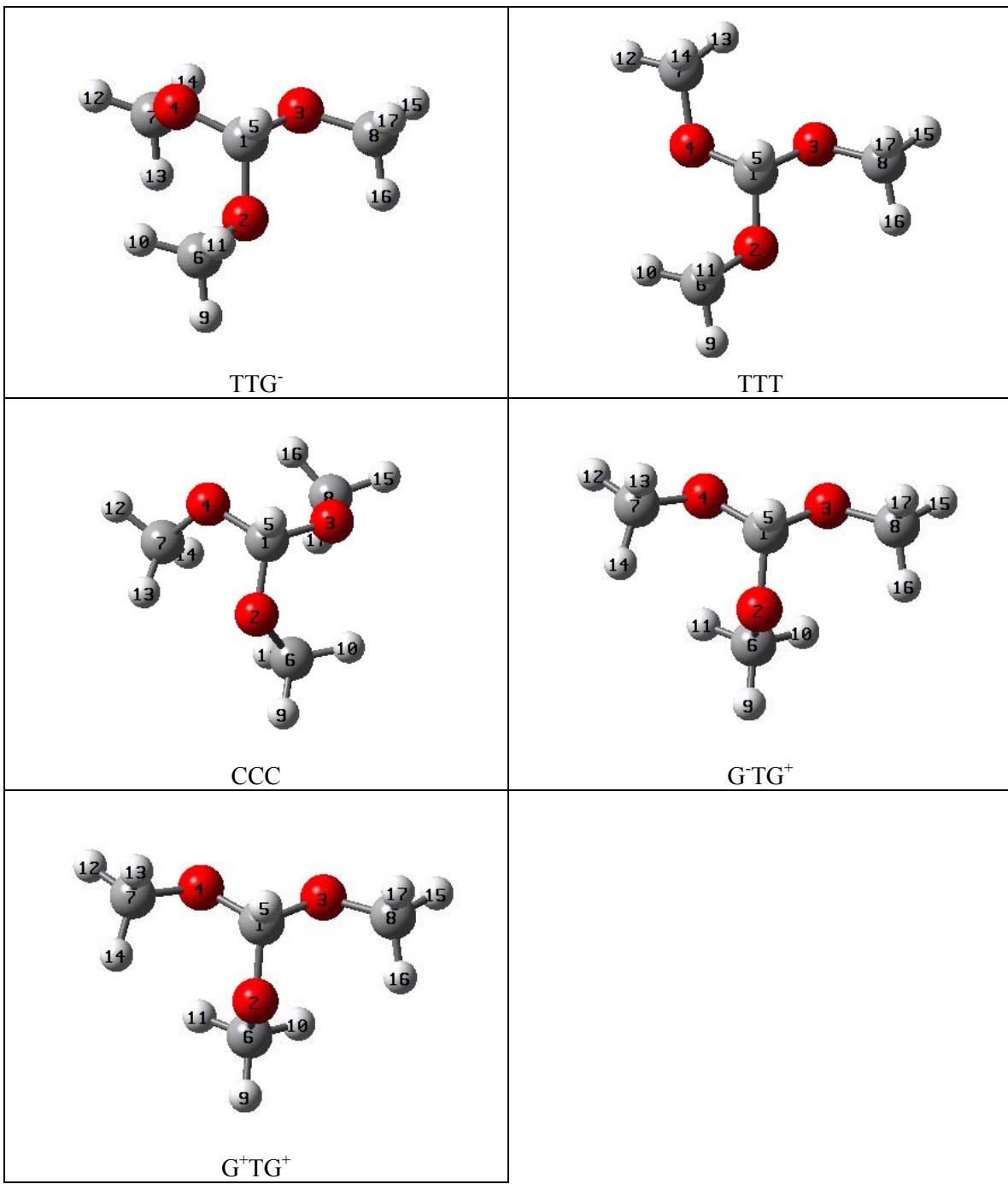


Figure 2: Stable conformations of Trimethoxymethane (3MM)

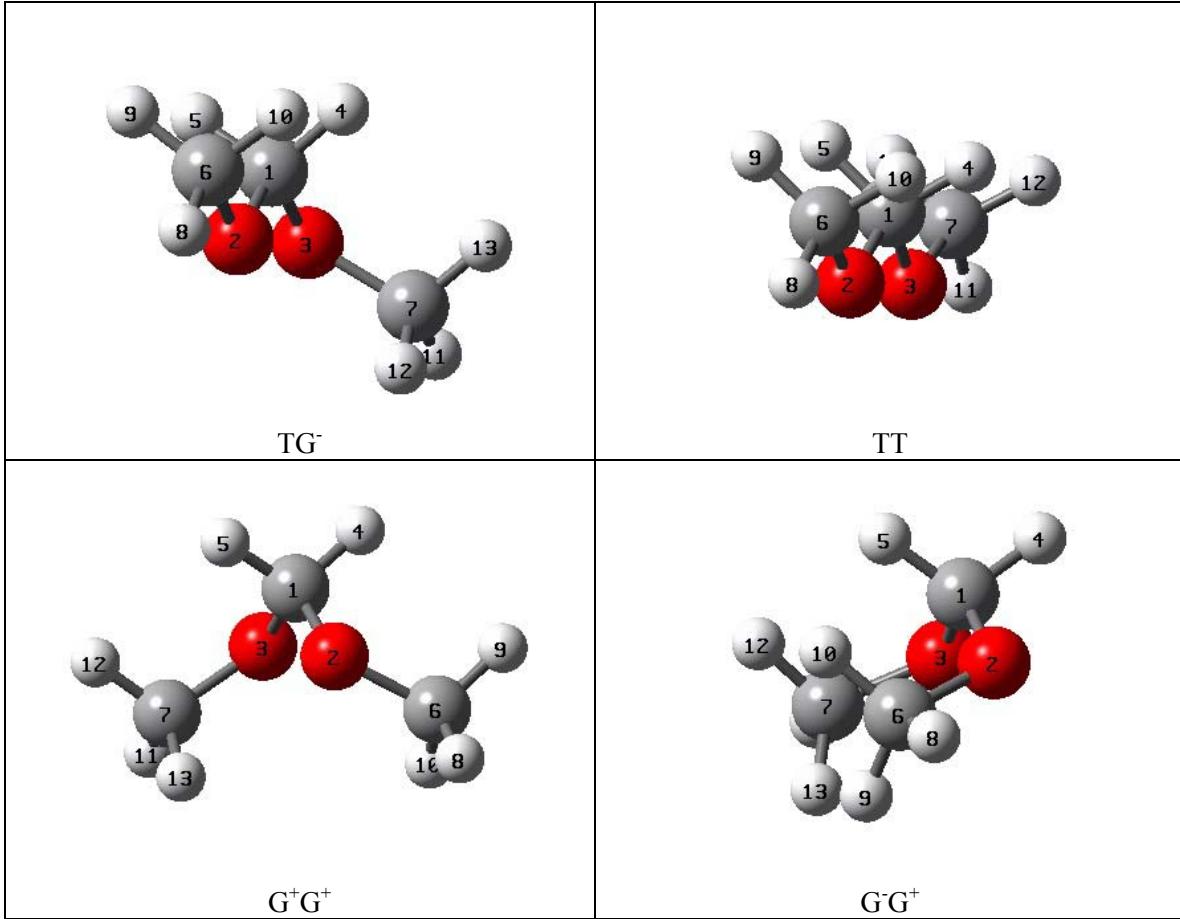


Figure 3: Stable conformations of Dimethoxymethane (2MM)

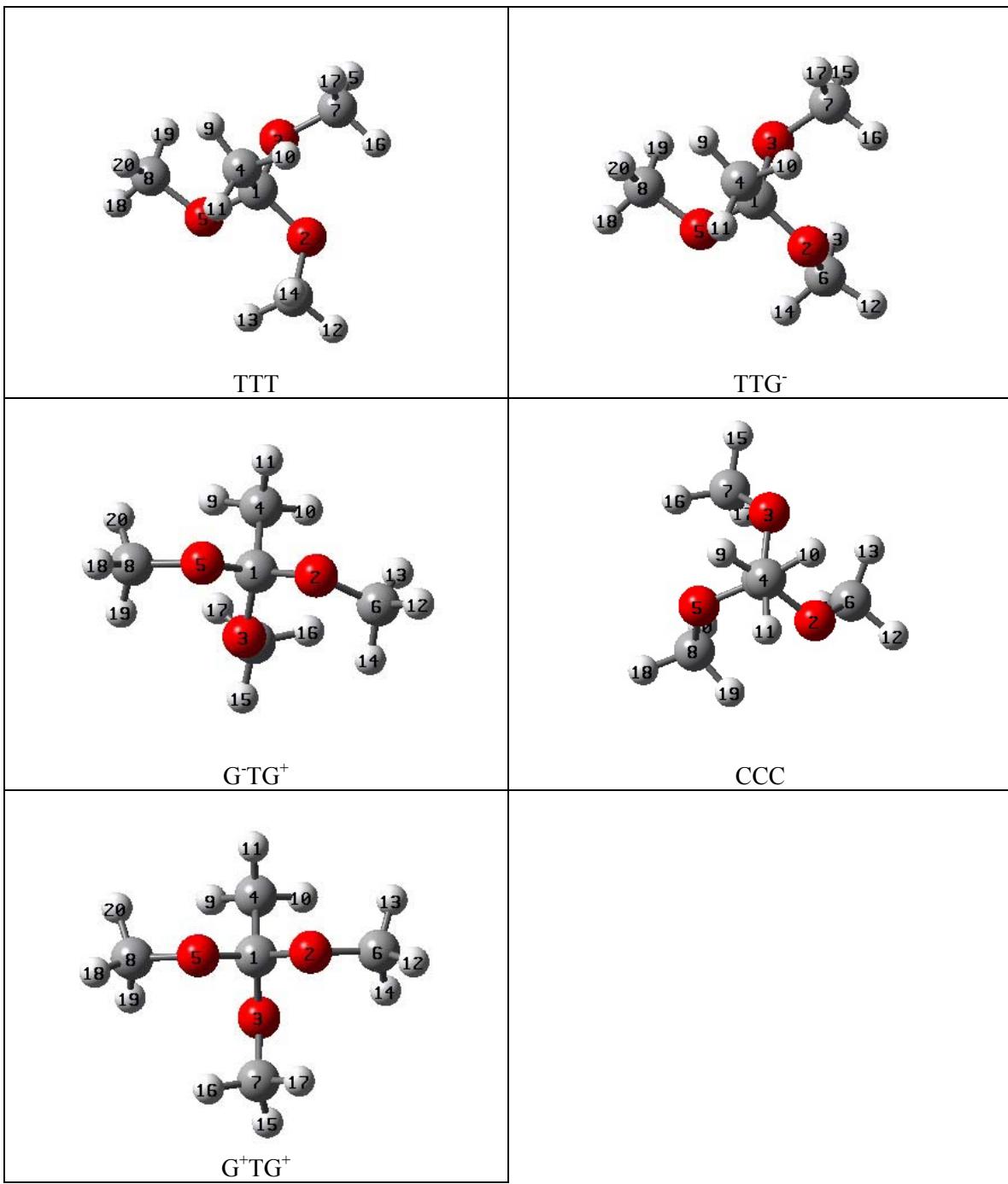


Figure 4: Stable Conformations of 1,1,1-Trimethoxyethane (3ME)

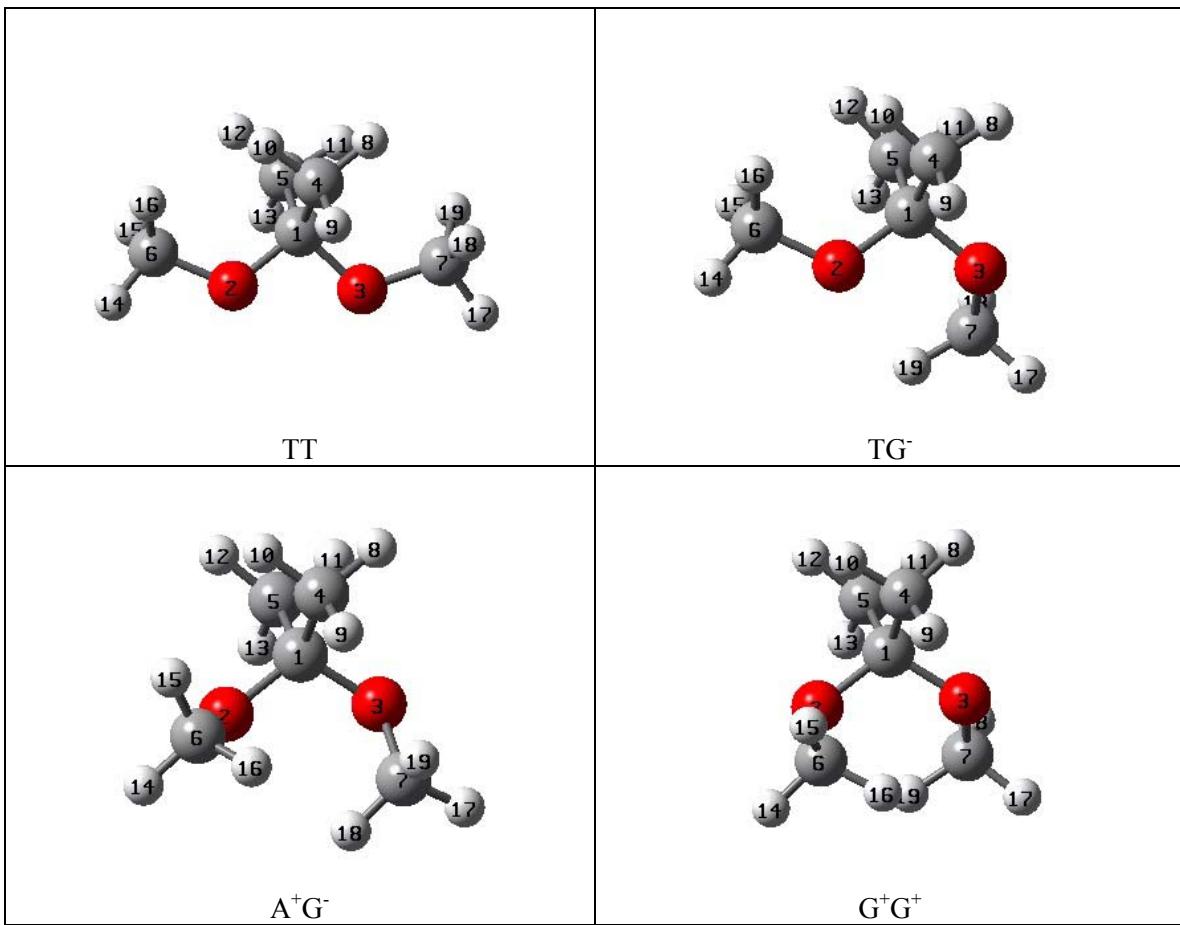


Figure 5: Stable Conformations of 2,2-Dimethoxypropane (2MP)

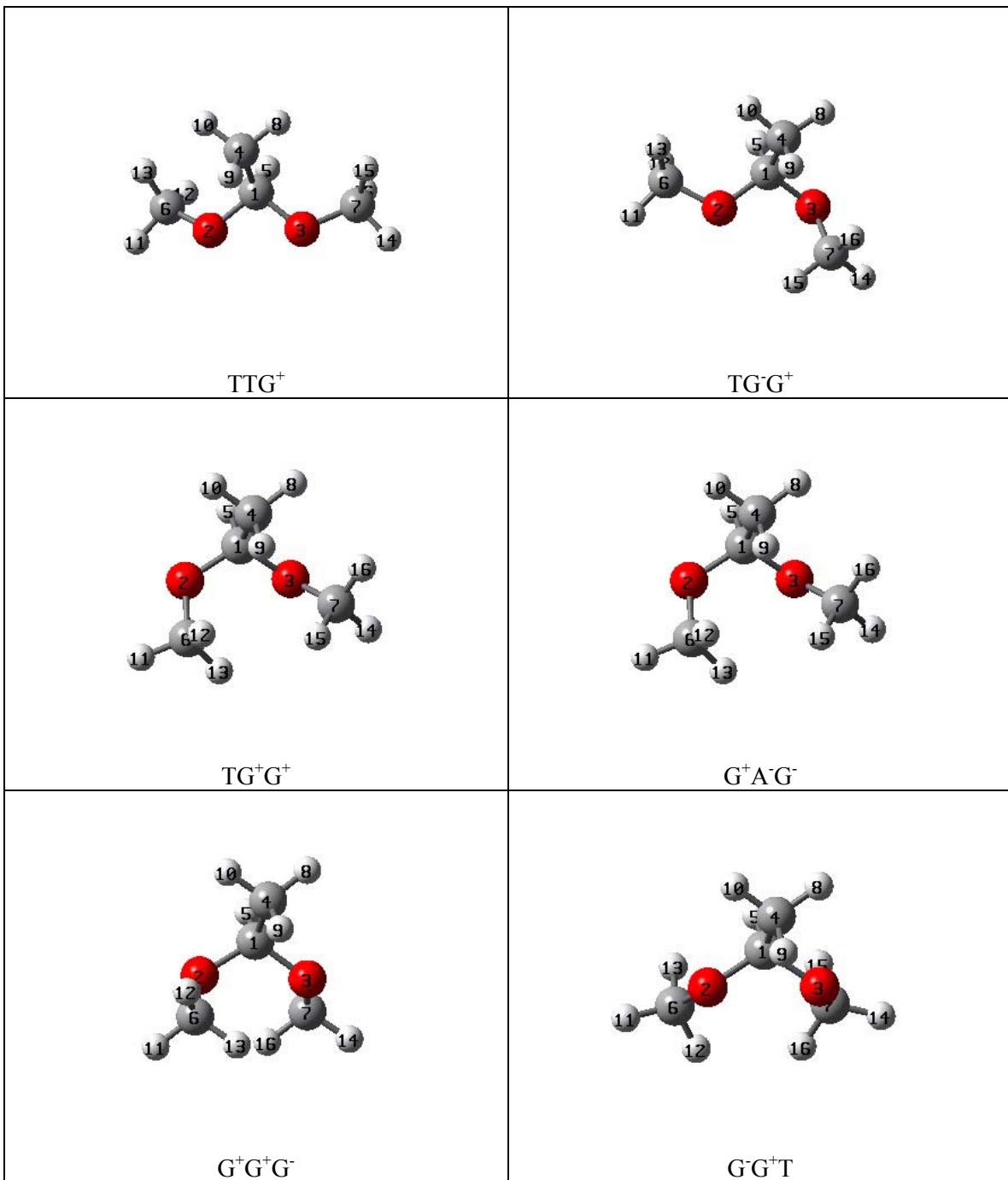


Figure 6: Stable conformations of 1,1-Dimethoxyethane (2ME)

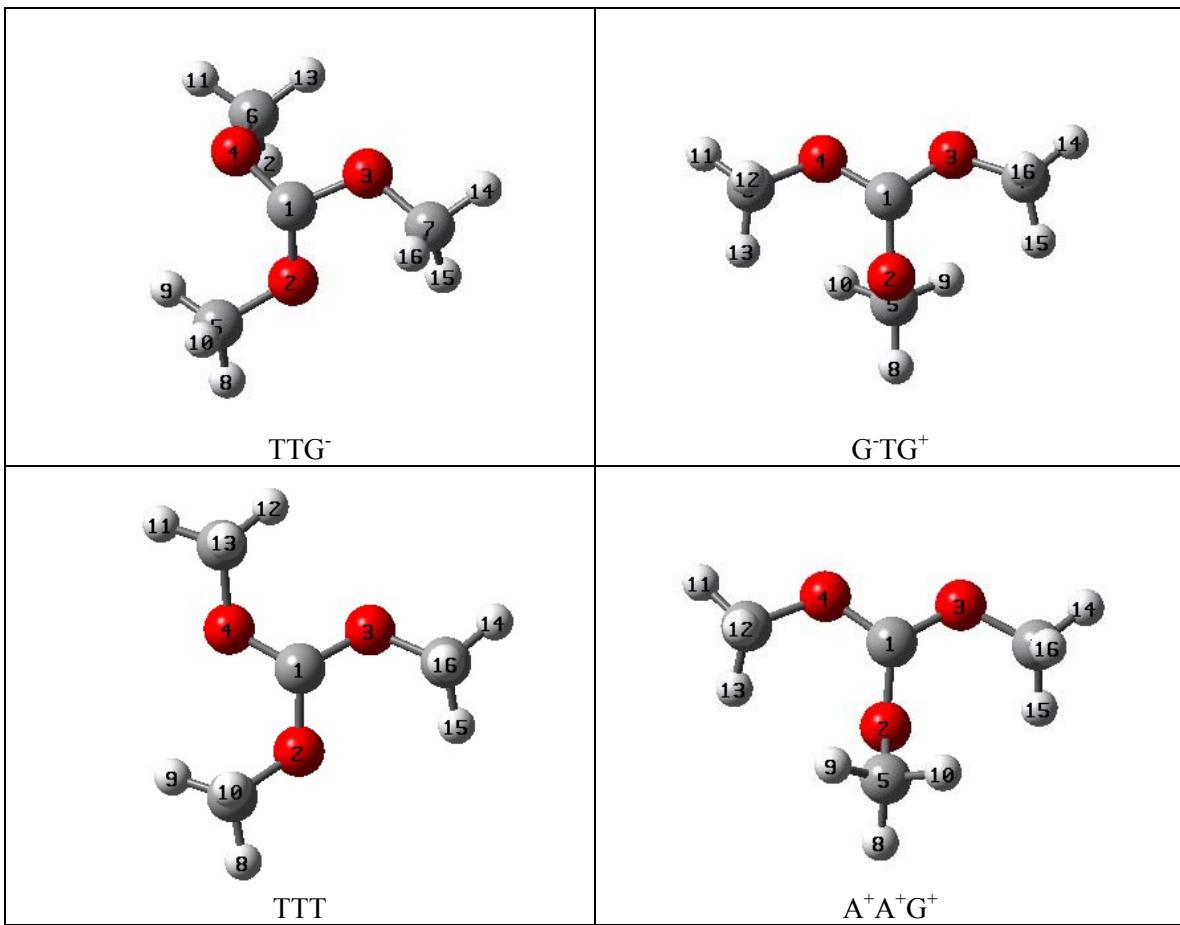


Figure 7: Stable conformations of Trimethoxymethyl radical (3MMR)

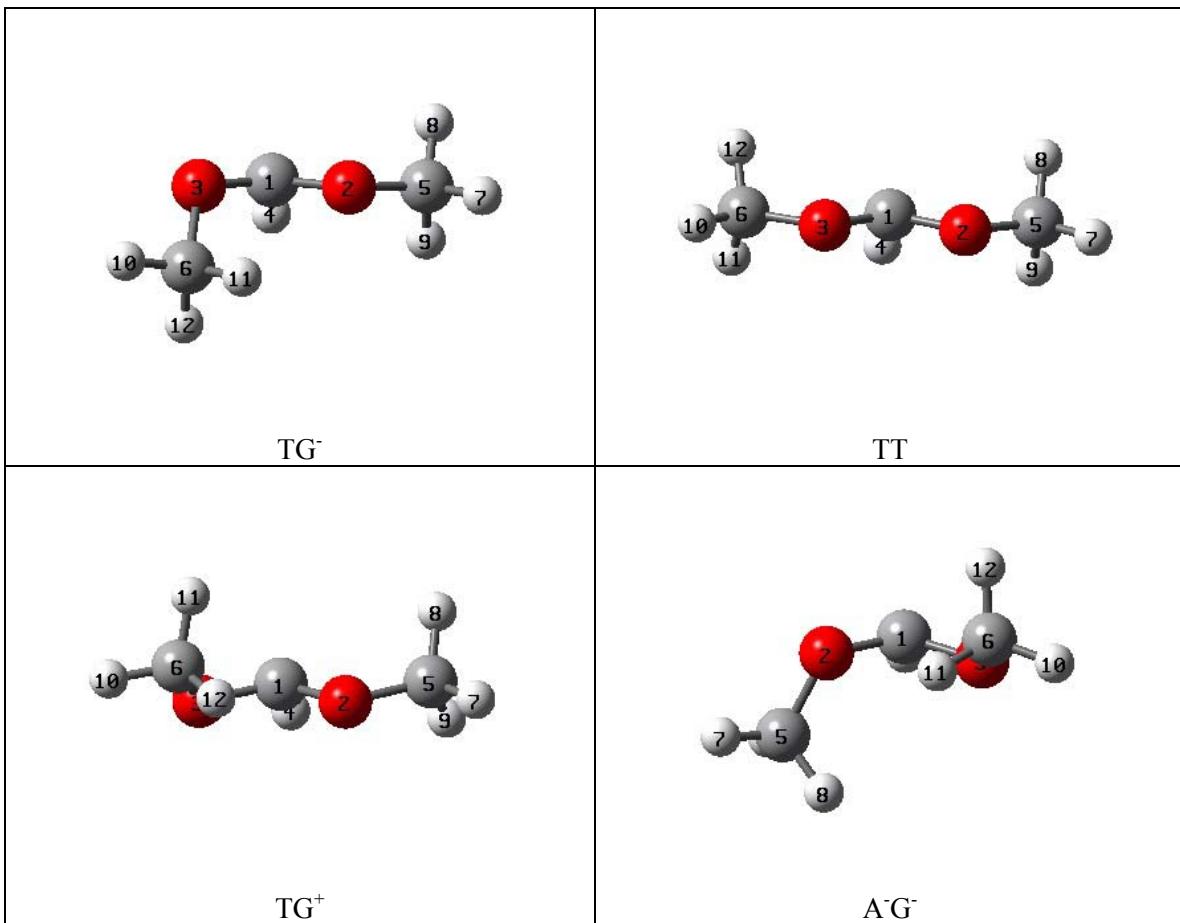


Figure 8: Stable conformations of Dimethoxymethyl radical (2MMR)

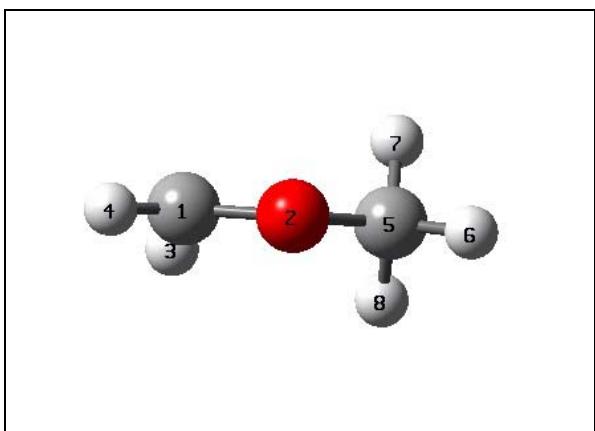


Figure 9: Methoxymethyl radical (MMR)

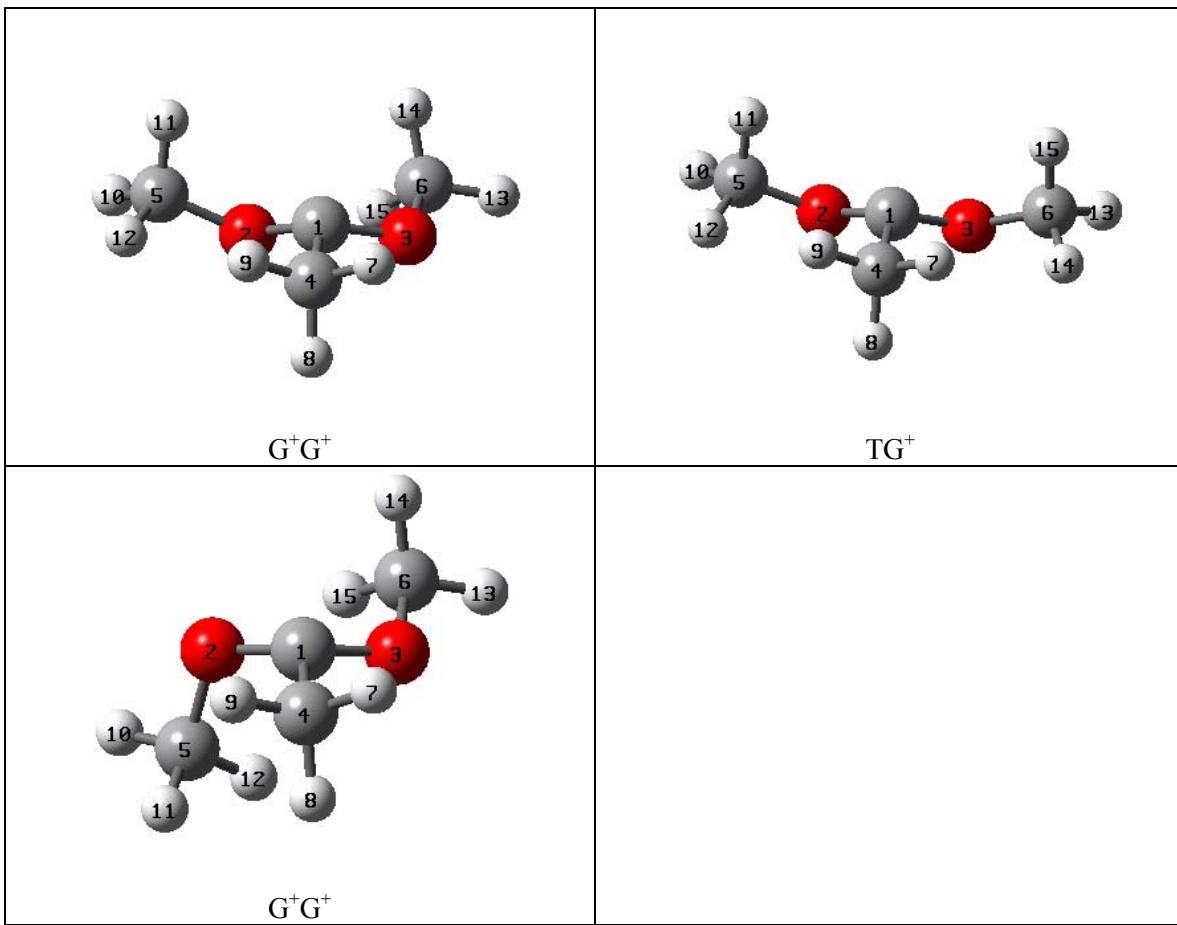


Figure 10: Stable conformations for 1,1-Dimethoxyethane 1-yl radical (2ME)

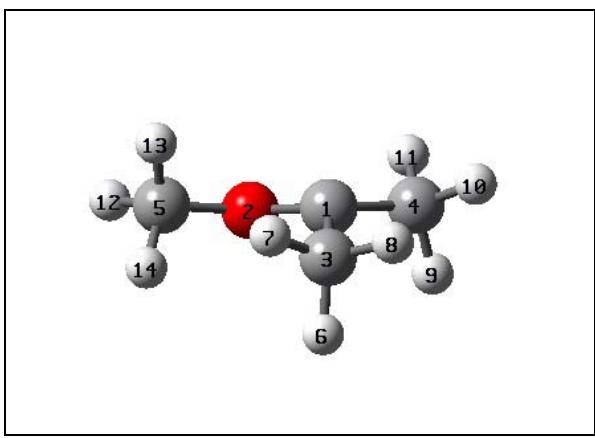


Figure 11: 2-Methoxypropane 2-yl radical (MPR)

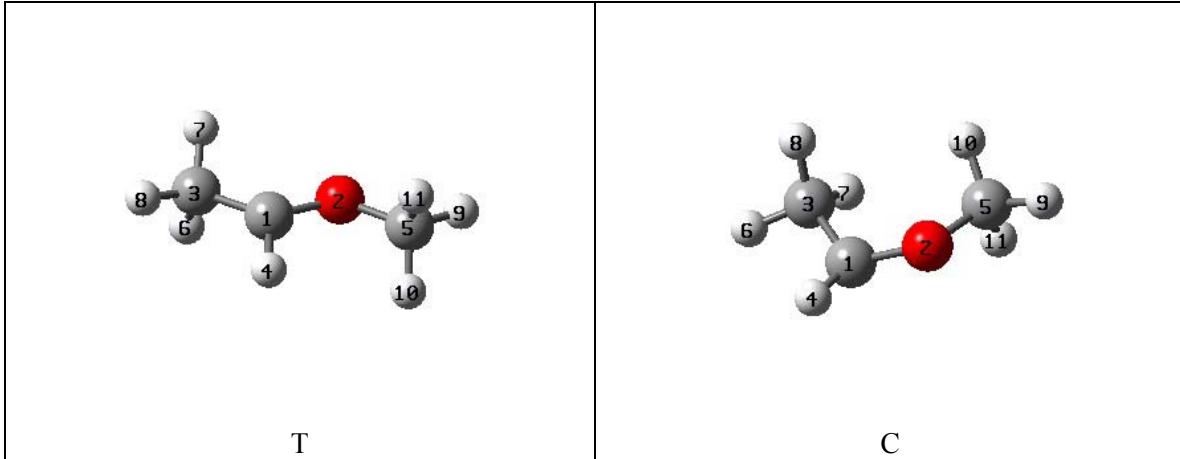


Figure 12: Stable conformations of 1-Methoxyethane 1-yl radical (MER)

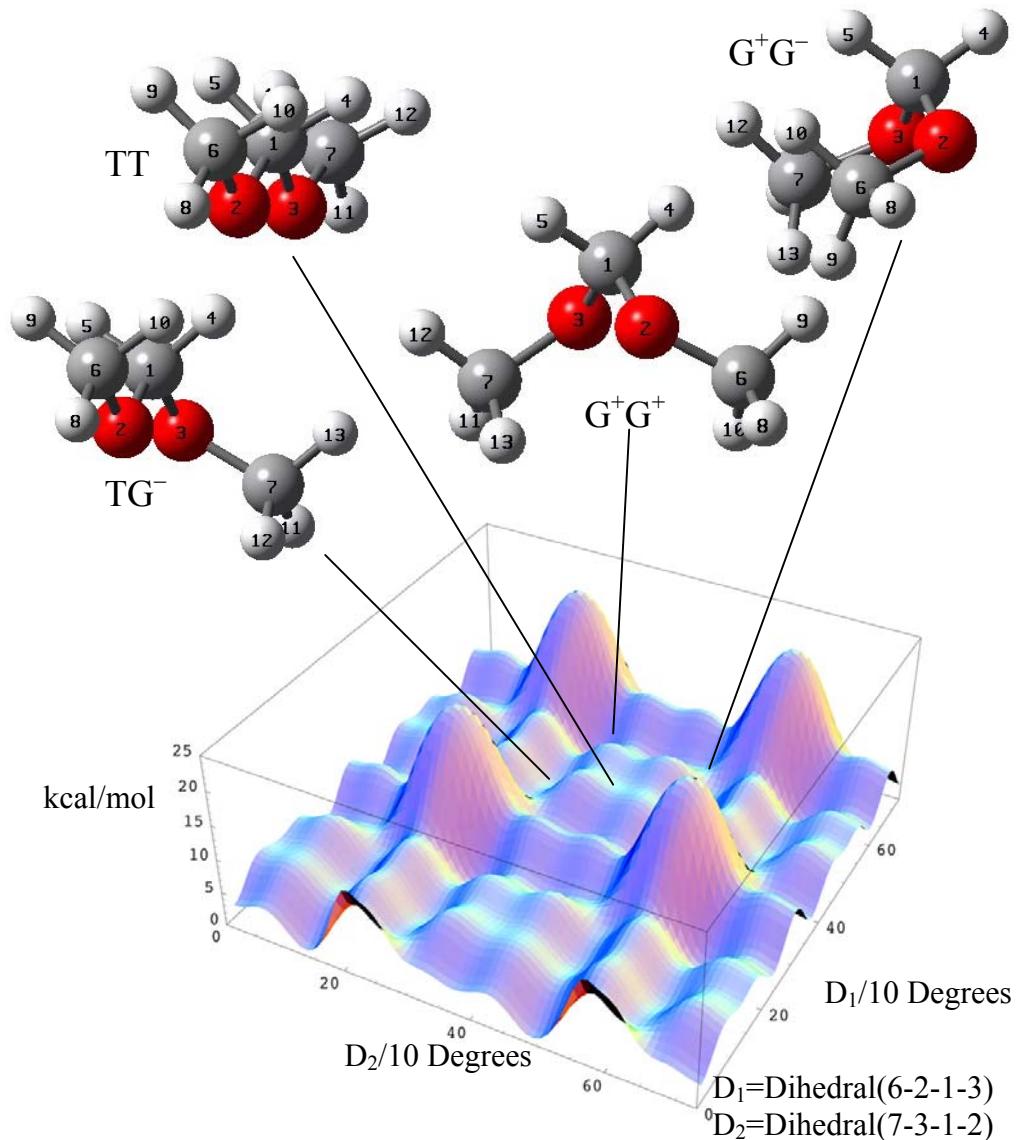


Figure 13: Energy landscape of dimethoxymethane. The energy relative to the lowest energy conformation (G^+G^+) is plotted versus the dihedral angle of the two methoxy groups.

Appendix A: Total Energies and Enthalpies of Formation for Species Used in the Isodesmic Reaction.

<i>Isodesmic Species</i>	<i>B3LYP (Hartrees)</i>	<i>B3LYP+ (Hartrees)</i>	<i>CBS-Q (Hartrees)</i>	<i>ZPVE kcal/mol</i>	$\Delta H_f(298, \text{Kcal/mol})$	<i>Unc.</i>	<i>Ref</i>
Ethane	-79.760838476	-79.783558346	-79.624721324	47.02	-20.400	0.070	[18]
Propane	-119.048186358	-119.081061425	-118.848598486	65.08	-25.020	0.120	[18]
Isobutane	-158.336817240	-158.379850095	-158.076209196	82.75	-32.070	0.150	[18]
Neopentane	-197.625230494	-197.678566645	-197.306458568	100.28	-40.140	0.150	[19]
Methanol	-115.669307685	-115.718016239	-115.534263160	32.26	-48.070	0.050	[20]
Ethanol	-154.962655260	-155.020714833	-154.762977773	50.30	-56.230	0.120	[20]
Isopropanol	-194.256108911	-194.323709726	-193.993719195	67.94	-65.070	0.220	[21]
t-Butanol	-233.548307802	-233.625544787	-233.241673616	85.23	-74.720	0.210	[22]
Dimethyl Ether	-154.949351063	-155.004527934	-154.744857291	50.14	-43.990	0.120	[23]
Methyl Ethyl Ether	-194.241996523	-194.306863771	-193.973656233	68.06	-51.730	0.160	[23]
Methyl Isopropyl Ether	-233.533009832	-233.607417056	-233.202859943	85.62	-60.240	0.230	[23]
Methyl t-Butyl Ether	-272.821448577	-272.906111938	-272.432842138	103.01	-67.679	0.306	[24]
Methyl Radical	-39.809672525	-39.824484701	-37.740159074	18.66	34.820	0.200	[25]
Ethyl Radical	-79.102022602	-79.126730312	-78.965355834	37.29	28.400	0.500	[26]
Isopropyl Radical	-118.395599817	-118.430164337	-118.193543640	55.37	22.000	0.500	[26]
t-Butyl Radical	-157.689155962	-157.733305748	-157.423443140	73.27	11.000	0.700	[26]
Methoxy Radical	-115.014643500	-115.059048838	-114.869066100	23.02	4.100	1.000	[26]

Appendix B: The coefficients a_i and b_i for the fitted torsional potential for each hindered internal rotor for each conformation of each species. Columns 1 and 2 list the species and conformations, respectively. (See the text for explanation on the notation). Column 3 lists the rotor axis bond by the two atom number identifiers (x-y). The atom identifiers can be located on Figures 1-12. Column 4 lists the degeneracy of the rotor of interest, while Columns 6-12 list the coefficient a_i and b_i .

Species	Conform.	Rotor	#	Coef	i=0	i=1 (7)	i=2 (8)	i=3 (9)	i=4 (10)	i=5	i=6
4MM	TTTT	1-3	4	a_i	6.47409	-3.33501	-0.82922	1.24066	-0.04252	-0.03442	-0.06299
		MeO		b_i		-3.16377	-1.22211	0.49305	0.12479	0.05041	-0.03266
	TTTT	3-5	4	a_i	0.55634	0.00000	0.00000	-0.20408	0.00000	0.00000	-0.06395
		Me		b_i		0.00000	0.00000	-0.53394	0.00000	0.00000	-0.00793
	$G^+G^-G^+G^-$	4-9	4	a_i	0.33828	0.00000	0.00000	0.38851	0.00000	0.00000	0.05557
		Me		b_i		0.00000	0.00000	-0.00295	0.00000	0.00000	-0.00084
	$G^+G^-G^+G^-$	1-4	4	a_i	4.92922	-0.10371	-3.38008	1.21699	-0.20060	0.09204	-0.12007
		OMe		b_i		-0.00136	0.00032	-0.00018	-0.00009	-0.00027	-0.00016
	$A^+G^+G^-G^+$	1-4	1	a_i	9.90619	7.72379	-0.27397	1.58682	-0.44490	0.02225	0.03615
		Ome		b_i		-0.02672	-0.14887	-0.04763	0.00705	0.01396	0.00611
	$A^+G^+G^-G^+$	4-9	1	a_i	0.35621	0.00000	0.00000	0.40348	0.00000	0.00000	0.04648
		Me		b_i		0.00000	0.00000	-0.01871	0.00000	0.00000	0.00264
	$A^+G^+G^-G^+$	1-3	2	a_i	0.94030	-2.21414	1.14665	1.18350	0.32046	0.00249	-0.14692
		OMe		b_i		-3.59351	0.71173	-0.15250	0.04326	-0.14368	-0.02148
	$A^+G^+G^-G^+$	3-6	2	a_i	0.71219	-0.00307	0.00029	0.73843	-0.00441	0.00401	0.04488
		Me		b_i		0.00297	-0.00443	0.09501	-0.00119	-0.00171	-0.00857
	$A^+G^+G^-G^+$	2-7	1	a_i	0.71955	0.00000	0.00000	0.71457	0.00000	0.00000	-0.00665
		Me		b_i		0.00000	0.00000	-0.05164	0.00000	0.00000	-0.00288
	$A^+G^+G^-G^+$	1-2	1	a_i	2.49543	-0.10371	-3.38008	1.21699	-0.20060	0.09204	-0.12007
		OMe		b_i		-0.00136	0.00032	-0.00018	-0.00009	-0.00027	-0.00016
3MM	TTG ⁻	2-6	1	a_i	0.73785	0.00000	0.00000	0.77689	0.00000	0.00000	0.03827
		Me		b_i		0.00000	0.00000	0.05191	0.00000	0.00000	0.00366

Species	Conform.	Rotor	#	Coef	i=0	i=1 (7)	i=2 (8)	i=3 (9)	i=4 (10)	i=5	i=6
	TTG ⁻	3-8	1	a _i	0.81820	0.00035	-0.00034	0.83820	-0.00032	0.00031	0.03842
		Me		b _i		0.00003	-0.00007	0.15322	-0.00013	0.00016	-0.01173
	TTG ⁻	4-7	1	a _i	0.51508	0.00000	0.00000	0.48849	0.00000	0.00000	0.03324
		Me		b _i		0.00000	0.00000	-0.19626	0.00000	0.00000	0.01325
	TTG ⁻	1-3	1	a _i	3.04593	-2.12889	0.41055	1.08654	0.29252	-0.12620	0.02848
		OMe		b _i		-1.34898	0.75433	-0.03000	-0.08208	0.05761	0.00082
	TTG ⁻	1-2	1	a _i	5.75525	3.30322	-0.96010	1.08549	-0.06373	0.11545	-0.02182
		OMe		b _i		-0.73642	2.19839	0.66651	0.03875	-0.06383	-0.09121
	TTG ⁻	1-4	1	a _i	2.46481	1.09134	0.11094	1.38722	0.12969	0.04466	-0.09536
		OMe		b _i		1.67547	1.33121	-0.30935	0.03310	0.10984	0.01809
	TTT	1-2	3	a _i	2.46481	1.09134	0.11094	1.38722	0.12969	0.04466	-0.09536
		OMe		b _i		1.67547	1.33121	-0.30935	0.03310	0.10984	0.01809
	TTT	2-6	3	a _i	0.79676	0.00389	0.00143	0.81606	-0.00302	-0.00331	0.03748
		Me		b _i		-0.00283	-0.00437	0.15160	-0.00235	-0.00024	-0.00033
	CCC	1-2	3	a _i	3.82412	-4.12470	-0.33209	1.62642	0.19837	-0.04457	0.05709
		OMe		b _i		4.49962	-2.72506	0.56599	-0.19995	0.06173	-0.02220
	CCC	2-6	3	a _i	0.93673	-0.00034	0.00033	0.88007	0.00028	-0.00024	0.04202
		Me		b _i		0.00006	-0.00011	-0.46676	-0.00021	0.00025	-0.03928
	G ⁻ TG ⁺	1-2	1	a _i	6.36085	0.96335	-4.31477	1.17429	0.00818	0.06874	0.02925
		OMe		b _i		-0.00344	0.00226	-0.00004	0.00036	0.00120	-0.00163
	G ⁻ TG ⁺	2-6	1	a _i	0.33938	0.00000	0.00000	0.39948	0.00000	0.00000	0.05799
		Me		b _i		0.00000	0.00000	-0.01214	0.00000	0.00000	-0.00522
	G ⁻ TG ⁺	1-3	2	a _i	2.32688	2.16794	0.34829	1.03711	-0.02180	0.13490	-0.01467
		OMe		b _i		1.35274	0.78526	0.22657	-0.32584	-0.02154	0.02609
	G ⁻ TG ⁺	3-8	2	a _i	0.76347	0.00000	0.00000	0.80845	0.00000	0.00000	0.04090
		Me		b _i		0.00000	0.00000	0.00125	0.00000	0.00000	-0.01078
	G ⁺ TG ⁺	4-7	2	a _i	0.27454	0.00000	0.00000	0.28117	0.00000	0.00000	0.00890
		Me		b _i		0.00000	0.00000	-0.00681	0.00000	0.00000	0.00085
	G ⁺ TG ⁺	3-8	1	a _i	1.05561	0.00035	-0.00035	1.11198	-0.00034	0.00033	0.05300
		Me		b _i		0.00002	-0.00005	0.09971	-0.00009	0.00011	-0.01142
	G ⁺ TG ⁺	1-2	2	a _i	-1.38969	1.08940	0.11355	1.39031	0.12983	0.04298	-0.09749
		OMe		b _i		1.67152	1.32860	-0.30850	0.03577	0.11126	0.01736
	G ⁺ TG ⁺	1-3	1	a _i	2.07095	0.96335	-4.31477	1.17429	0.00818	0.06874	0.02925
		OMe		b _i		-0.00344	0.00226	-0.00004	0.00036	0.00120	-0.00163
2MM	TG ⁻	3-7	1	a _i	0.79310	0.00035	-0.00034	0.82346	-0.00033	0.00032	0.04025
		Me		b _i		0.00003	-0.00005	0.12204	-0.00010	0.00013	-0.00445
	TG ⁻	2-6	1	a _i	1.14730	0.00000	0.00000	1.18986	0.00000	0.00000	0.04677
		Me		b _i		0.00000	0.00000	0.06521	0.00000	0.00000	0.02323
	TG ⁻	1-3	1	a _i	2.66712	0.24280	-0.71897	1.49530	-0.07630	0.01280	0.00257
		OMe		b _i		-0.44837	-1.34156	0.05906	0.07422	0.00838	0.00176
	TG ⁻	1-2	1	a _i	1.58753	-2.62728	0.58609	1.28513	-0.03354	-0.04208	0.00743
		OMe		b _i		-0.83988	2.39222	-0.30470	0.00787	-0.01135	0.05603
	TT	1-3	2	a _i	-0.62987	-0.46053	1.55444	1.47846	0.06908	-0.03758	-0.01902
		OMe		b _i		0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
	TT	3-7	2	a _i	1.21176	0.01851	0.02635	1.24234	-0.02420	-0.01290	0.03532
		Me		b _i		-0.00027	0.00001	-0.00038	0.00029	-0.00018	-0.00018
	G ⁺ G ⁺	1-3	2	a _i	4.39425	-2.62728	0.58609	1.28513	-0.03354	-0.04208	0.00743
		OMe		b _i		-0.83988	2.39222	-0.30470	0.00787	-0.01135	0.05603
	G ⁺ G ⁺	3-7	2	a _i	0.77393	0.00000	0.00000	0.81384	0.00000	0.00000	0.03829
		OMe		b _i		0.00000	0.00000	-0.07327	0.00000	0.00000	-0.01176
	G ⁻ G ⁺	3-7	2	a _i	0.78857	0.00000	0.00000	0.46674	0.00000	0.00000	-0.00394
		Me		b _i		0.00000	0.00000	-0.68478	0.00000	0.00000	-0.03542
	G ⁻ G ⁺	1-3	2	a _i	0.36748	-2.62728	0.58609	1.28513	-0.03354	-0.04208	0.00743
		OMe		b _i		-0.83988	2.39222	-0.30470	0.00787	-0.01135	0.05603
3ME	TTT	1-4	1	a _i	1.33132	0.00069	-0.00066	1.28847	-0.00054	0.00045	0.10648
		Me		b _i		-0.00012	0.00024	-0.59446	0.00045	-0.00053	-0.05065
	TTT	1-5	3	a _i	-4.62527	2.09837	0.74540	1.29128	0.06027	0.11682	-0.00509

Species	Conform.	Rotor	#	Coef	i=0	i=1 (7)	i=2 (8)	i=3 (9)	i=4 (10)	i=5	i=6
		OMe		b _i		4.24080	2.02924	0.36601	-0.15848	-0.06101	0.02200
	TTT	5-8	3	a _i	0.63982	-0.00005	0.00046	0.63597	0.00010	0.00004	0.03862
		Me		b _i		0.00036	-0.00029	-0.21949	0.00040	-0.00009	-0.00012
	TTG ⁻	1-4	1	a _i	1.38150	0.00109	-0.00071	1.41736	0.00123	-0.00145	0.07465
		Me		b _i		0.00046	-0.00101	-0.35104	-0.00058	-0.00087	-0.03573
	TTG ⁻	1-5	1	a _i	2.77049	1.77739	0.26331	1.04012	-0.02811	0.13723	0.01668
		OMe		b _i		0.03106	-1.35589	-0.17389	0.21301	0.00865	-0.05460
	TTG ⁻	5-8	1	a _i	0.58202	0.00000	0.00000	0.62667	0.00000	0.00000	0.03906
		Me		b _i		0.00000	0.00000	-0.06872	0.00000	0.00000	-0.02214
	TTG ⁻	1-3	1	a _i	5.35209	-1.77706	1.51969	1.15674	0.04903	-0.09977	-0.03534
		OMe		b _i		2.98017	-0.23771	0.63741	-0.01822	-0.08566	0.01468
	TTG ⁻	3-7	1	a _i	0.76518	0.00011	-0.00010	0.58993	-0.00007	0.00004	0.02111
		Me		b _i		-0.00003	0.00005	-0.45957	0.00010	-0.00011	0.01899
	TTG ⁻	2-6	1	a _i	0.47377	0.00000	0.00000	0.47517	0.00000	0.00000	0.05152
		Me		b _i		0.00000	0.00000	-0.14155	0.00000	0.00000	0.01921
	TTG ⁻	1-2	1	a _i	6.26839	2.09837	0.74540	1.29128	0.06027	0.11682	-0.00509
		OMe		b _i		4.24080	2.02924	0.36601	-0.15848	-0.06101	0.02200
	G ⁺ TG ⁺	1-4	1	a _i	1.76121	0.00000	0.00000	1.86280	0.00000	0.00000	0.15100
		Me		b _i		0.00000	0.00000	0.51775	0.00000	0.00000	0.14047
	G ⁺ TG ⁺	1-5	2	a _i	0.47836	-1.32549	-0.10548	1.53560	-0.05929	0.01577	-0.00363
		OMe		b _i		2.19761	0.07962	-0.17313	-0.05470	-0.00339	0.01766
	G ⁺ TG ⁺	5-8	2	a _i	0.71399	0.00017	0.00021	0.73240	-0.00002	0.00034	0.04932
		Me		b _i		-0.00032	0.00026	-0.19708	-0.00033	0.00012	-0.00554
	G ⁺ TG ⁺	1-3	1	a _i	2.03552	-0.12259	2.03446	1.30930	0.11964	-0.04143	-0.01068
		OMe		b _i		-1.41053	-4.03704	-0.32512	0.25854	0.11852	-0.03204
	G ⁺ TG ⁺	3-7	1	a _i	0.80618	0.00035	-0.00035	0.80451	-0.00035	0.00035	-0.00719
		Me		b _i		0.00000	0.00000	-0.02844	0.00002	-0.00002	-0.00034
	CCC	1-4	1	a _i	1.89630	0.00069	-0.00067	1.76486	-0.00061	0.00056	0.03606
		Me		b _i		0.00009	-0.00018	0.79981	-0.00034	0.00042	0.02867
	CCC	1-3	3	a _i	3.98356	-3.23920	-2.29889	1.26620	-0.03152	0.22516	0.07028
		OMe		b _i		-5.58608	1.34366	0.11495	0.54747	0.08221	-0.07217
	CCC	3-7	3	a _i	0.93372	0.00038	0.00014	0.82980	0.00054	-0.00013	-0.00175
		Me		b _i		0.00048	-0.00059	-0.50138	0.00027	-0.00059	-0.04312
	G ⁺ TG ⁺	1-4	1	a _i	1.49514	0.00013	-0.00036	1.55847	-0.00042	0.00018	0.07800
		Me		b _i		0.00022	-0.00025	0.22453	0.00014	-0.00018	0.03749
	G ⁺ TG ⁺	5-8	2	a _i	0.71798	0.00000	0.00000	0.55247	0.00000	0.00000	0.03920
		Me		b _i		0.00000	0.00000	-0.45064	0.00000	0.00000	0.00516
	G ⁺ TG ⁺	3-7	1	a _i	0.71955	0.00000	0.00000	0.55398	0.00000	0.00000	0.03710
		Me		b _i		0.00000	0.00000	0.44451	0.00000	0.00000	-0.00801
	G ⁺ TG ⁺	1-5	2	a _i	1.52702	1.77739	0.26331	1.04012	-0.02811	0.13723	0.01668
		OMe		b _i		0.03106	-1.35589	-0.17389	0.21301	0.00865	-0.05460
	G ⁺ TG ⁺	1-3	1	a _i	7.52979	-0.12259	2.03446	1.30930	0.11964	-0.04143	-0.01068
		OMe		b _i		-1.41053	-4.03704	-0.32512	0.25854	0.11852	-0.03204
2MP	TT	1-4	1	a _i	1.88915	0.00035	-0.00035	1.89507	-0.00035	0.00035	0.02496
		Me		b _i		0.00000	0.00001	-0.20109	0.00001	-0.00001	-0.05106
	TT	1-3	2	a _i	-1.47486	-2.12265	0.58502	1.51619	0.01372	-0.13430	0.11236
		OMe		b _i		-0.00045	0.00096	-0.00175	0.00218	-0.00165	0.00114
	TT	3-7	2	a _i	0.80984	0.00035	-0.00034	0.85094	-0.00032	0.00031	0.07908
		Me		b _i		0.00004	-0.00007	0.12228	-0.00014	0.00017	-0.02691
	TT	1-5	1	a _i	1.44572	0.00793	-0.00495	1.52353	0.00300	-0.00574	0.11505
		Me		b _i		-0.00364	0.00617	0.46277	0.00529	-0.00202	0.09870
	TG ⁻	1-5	1	a _i	1.41151	-0.00002	-0.00001	1.41230	-0.00003	0.00000	0.04463
		Me		b _i		-0.00003	0.00004	-0.40450	-0.00003	0.00004	-0.04979
	TG ⁻	1-4	1	a _i	1.54472	0.00000	0.00000	1.34113	0.00000	0.00000	0.06951
		Me		b _i		0.00000	0.00000	0.78131	0.00000	0.00000	-0.00678
	TG ⁻	1-2	1	a _i	0.53658	-0.11312	0.44895	1.16353	0.18035	0.17415	0.01817
		OMe		b _i		-1.53755	-1.18278	0.06324	0.27334	-0.04809	-0.17298

Species	Conform.	Rotor	#	Coef	i=0	i=1 (7)	i=2 (8)	i=3 (9)	i=4 (10)	i=5	i=6
	TG ⁻	2-6	1	a _i	0.82727	0.00000	0.00000	0.85760	0.00000	0.00000	0.05179
		Me		b _i		0.00000	0.00000	0.10221	0.00000	0.00000	-0.03090
	TG ⁻	3-7	1	a _i	0.69004	0.00040	0.00066	0.65287	0.00063	0.00046	0.03851
		Me		b _i		-0.00095	0.00096	0.29307	-0.00084	0.00081	0.00298
	TG ⁻	1-3	1	a _i	2.83488	-2.12265	0.58502	1.51619	0.01372	-0.13430	0.11236
		OMe		b _i		-0.00045	0.00096	-0.00175	0.00218	-0.00165	0.00114
	A ⁺ G ⁻	1-4	1	a _i	1.85830	0.00035	-0.00035	1.89821	-0.00034	0.00033	0.05725
		Me		b _i		0.00002	-0.00004	0.25904	-0.00008	0.00010	0.01283
	A ⁺ G ⁻	1-5	1	a _i	1.60294	-0.00035	0.00033	1.54000	0.00029	-0.00026	0.05138
		Me		b _i		-0.00005	0.00010	0.60116	0.00019	-0.00023	0.02131
	A ⁺ G ⁻	3-7	1	a _i	1.22608	0.00035	-0.00035	1.26313	-0.00035	0.00035	0.02049
		Me		b _i		0.00000	0.00000	0.07821	-0.00001	0.00001	0.05947
	A ⁺ G ⁻	2-6	1	a _i	0.83518	-0.00118	0.00042	0.78701	-0.00124	0.00149	-0.03179
		Me		b _i		0.00088	-0.00142	0.13242	-0.00084	-0.00005	-0.01636
	A ⁺ G ⁻	1-3	2	a _i	-0.80628	-0.11312	0.44895	1.16353	0.18035	0.17415	0.01817
		OMe		b _i		-1.53755	-1.18278	0.06324	0.27334	-0.04809	-0.17298
	G ⁺ G ⁺	1-5	2	a _i	1.55683	0.01071	-0.00865	1.50406	-0.00259	-0.00014	0.05028
		Me		b _i		-0.00359	0.00652	0.54499	0.00867	-0.00781	0.01610
	G ⁺ G ⁺	3-7	2	a _i	0.79589	0.00000	0.00000	0.64575	0.00000	0.00000	0.02718
		Me		b _i		0.00000	0.00000	0.47638	0.00000	0.00000	-0.00201
	G ⁺ G ⁺	1-3	2	a _i	3.99695	-0.11312	0.44895	1.16353	0.18035	0.17415	0.01817
		OMe		b _i		-1.53755	-1.18278	0.06324	0.27334	-0.04809	-0.17298
2ME	TTG ⁺	1-4	1	a _i	1.48458	0.00000	0.00000	1.51948	0.00000	0.00000	0.04485
		Me		b _i		0.00000	0.00000	-0.19885	0.00000	0.00000	-0.02589
	TTG ⁺	3-7	2	a _i	0.94650	0.00000	0.00000	0.98240	0.00000	0.00000	0.04298
		Me		b _i		0.00000	0.00000	0.19766	0.00000	0.00000	0.01620
	TTG ⁺	1-3	2	a _i	-0.51579	-1.35121	0.99486	1.43236	0.00171	-0.01134	0.02168
		OMe		b _i		-1.64354	0.12437	-0.08953	0.10640	0.03121	-0.01760
	TG ⁻ G ⁺	1-4	1	a _i	1.42846	0.00035	-0.00035	1.43149	-0.00034	0.00034	0.04131
		Me		b _i		-0.00002	0.00004	-0.32319	0.00008	-0.00009	-0.02361
	TG ⁻ G ⁺	3-7	1	a _i	0.67204	0.01257	0.02216	0.66754	-0.01869	-0.00422	0.02889
		Me		b _i		0.00289	-0.00276	-0.20182	0.01081	0.00882	-0.00375
	TG ⁻ G ⁺	2-6	1	a _i	0.89943	0.00000	0.00000	0.90128	0.00000	0.00000	0.02394
		Me		b _i		0.00000	0.00000	-0.23053	0.00000	0.00000	-0.01497
	TG ⁻ G ⁺	1-3	1	a _i	1.15983	-1.35121	0.99486	1.43236	0.00171	-0.01134	0.02168
		OMe		b _i		-1.64354	0.12437	-0.08953	0.10640	0.03121	-0.01760
	TG ⁻ G ⁺	1-2	1	a _i	1.00071	0.21308	0.94466	1.12176	0.18267	0.16625	-0.03154
		OMe		a _i		-0.07492	0.02329	0.04503	-0.01822		
				b _i		-2.99084	-0.74091	-0.18850	0.28602	-0.04007	-0.10797
				b _i		0.03337	0.05115	-0.01716	-0.03839		
	TG ⁺ G ⁺	1-4	1	a _i	1.44903	0.00000	0.00000	1.47660	0.00000	0.00000	0.02735
		Me		b _i		0.00000	0.00000	-0.04382	0.00000	0.00000	-0.02131
	TG ⁺ G ⁺	3-7	1	a _i	0.83703	0.00035	-0.00035	0.88153	-0.00034	0.00034	0.04323
		Me		b _i		-0.00001	0.00003	-0.05921	0.00006	-0.00007	0.00572
	TG ⁺ G ⁺	2-6	1	a _i	0.88723	0.00035	-0.00034	0.88857	-0.00032	0.00031	0.02305
		Me		b _i		-0.00003	0.00007	-0.24635	0.00013	-0.00016	-0.02048
	TG ⁺ G ⁺	1-3	1	a _i	4.08770	-1.35121	0.99486	1.43236	0.00171	-0.01134	0.02168
		OMe		b _i		-1.64354	0.12437	-0.08953	0.10640	0.03121	-0.01760
	TG ⁺ G ⁺	1-2	1	a _i	2.10841	0.26833	1.07223	1.19308	-0.09248	-0.00557	0.03553
		OMe		b _i		-0.14161	1.37227	0.04879	0.02713	-0.01740	-0.00439
	G ⁺ A ⁻ G ⁻	1-4	1	a _i	1.79660	0.00035	-0.00034	1.77198	-0.00032	0.00031	0.03190
		Me		b _i		0.00003	-0.00007	0.53117	-0.00013	0.00016	0.03641
	G ⁺ A ⁻ G ⁻	1-3	1	a _i	-1.73782	0.21308	0.94466	1.12176	0.18267	0.16625	-0.03154
		OMe		a _i		-0.07492	0.02329	0.04503	-0.01822		
				b _i		-2.99084	-0.74091	-0.18850	0.28602	-0.04007	-0.10797
				b _i		0.03337	0.05115	-0.01716	-0.03839		
	G ⁺ A ⁻ G ⁻	3-7	1	a _i	0.74970	0.00035	-0.00035	0.72444	-0.00034	0.00034	-0.01690

Species	Conform.	Rotor	#	Coef	i=0	i=1 (7)	i=2 (8)	i=3 (9)	i=4 (10)	i=5	i=6
		Me		b _i		-0.00002	0.00003	-0.14782	0.00007	-0.00008	0.01056
	G ⁺ A ⁻ G ⁻	1-2	1	a _i	-1.72645	0.20937	0.93767	1.12774	0.19699	0.16822	-0.04491
		OMe		b _i		2.99433	0.73480	0.17730	-0.28362	0.05524	0.11287
	G ⁺ A ⁻ G ⁻	2-6	1	a _i	0.73297	0.00191	-0.00191	0.75192	-0.00188	0.00185	-0.01593
		Me		b _i		-0.00010	0.00020	0.12358	0.00039	-0.00049	0.03168
	G ⁺ G ⁺ G ⁻	1-4	1	a _i	1.49661	0.00000	0.00000	1.36780	0.00000	0.00000	0.01809
		Me		b _i		0.00000	0.00000	0.70994	0.00000	0.00000	0.04216
	G ⁺ G ⁺ G ⁻	2-6	1	a _i	0.75040	0.00000	0.00000	0.64233	0.00000	0.00000	0.03165
		Me		b _i		0.00000	0.00000	0.41278	0.00000	0.00000	-0.00013
	G ⁺ G ⁺ G ⁻	3-7	1	a _i	0.74831	0.00000	0.00000	0.78778	0.00000	0.00000	0.03556
		Me		b _i		0.00000	0.00000	-0.01048	0.00000	0.00000	0.00014
	G ⁺ G ⁺ G ⁻	1-3	1	a _i	5.08488	0.21308	0.94466	1.12176	0.18267	0.16625	-0.03154
		OMe		a _i		-0.07492	0.02329	0.04503	-0.01822		
				b _i		-2.99084	-0.74091	-0.18850	0.28602	-0.04007	-0.10797
				b _i		0.03337	0.05115	-0.01716	-0.03839		
	G ⁺ G ⁺ G ⁻	1-2	1	a _i	3.25527	0.26833	1.07223	1.19308	-0.09248	-0.00557	0.03553
		OMe		b _i		-0.14161	1.37227	0.04879	0.02713	-0.01740	-0.00439
	G ⁻ G ⁺ T	1-4	1	a _i	1.39621	0.00000	0.00000	1.47023	0.00000	0.00000	0.07356
		Me		b _i		0.00000	0.00000	-0.00950	0.00000	0.00000	-0.00120
	G ⁻ G ⁺ T	1-3	1	a _i	2.48158	-1.77766	0.54934	-0.12184	0.01951	-0.01435	-0.00848
		OMe		b _i		-1.28990	0.32935	0.62388	0.01225	0.00320	-0.00309
	G ⁻ G ⁺ T	3-7	1	a _i	0.68712	0.00000	0.00000	0.36652	0.00000	0.00000	-0.03593
		OMe		b _i		0.00000	0.00000	-0.65472	0.00000	0.00000	-0.05228
	G ⁻ G ⁺ T	1-2	1	a _i	1.00347	0.05652	0.66199	1.21577	-0.03667	-0.00648	0.03980
		OMe		b _i		0.27231	-1.58931	0.06233	-0.04888	0.02164	-0.00238
	G ⁻ G ⁺ T	2-6	1	a _i	0.75824	0.00000	0.00000	0.44731	0.00000	0.00000	-0.01190
		Me		b _i		0.00000	0.00000	0.67080	0.00000	0.00000	0.04389
3MMR	TTG ⁻	2-5	1	a _i	0.52188	0.00000	0.00000	0.55509	0.00000	0.00000	0.03591
		Me		b _i		0.00000	0.00000	-0.06424	0.00000	0.00000	-0.00448
	TTG ⁻	4-6	1	a _i	0.52345	0.00000	0.00000	0.52000	0.00000	0.00000	0.02722
		Me		b _i		0.00000	0.00000	-0.14150	0.00000	0.00000	0.01096
	TTG ⁻	3-7	1	a _i	0.58672	0.00000	0.00000	0.58090	0.00000	0.00000	0.02061
		Me		b _i		0.00000	0.00000	0.14056	0.00000	0.00000	-0.02038
	TTG ⁻	1-2	1	a _i	5.64104	4.08557	-0.54362	0.74703	-0.04570	0.02962	-0.05447
		OMe		b _i		-0.75720	1.22925	0.35194	0.03527	-0.05363	-0.02537
	TTG ⁻	1-4	1	a _i	2.26413	2.92960	0.27610	0.65743	-0.01192	0.00629	-0.04712
		OMe		b _i		1.69572	1.29940	-0.06945	-0.05262	-0.06773	-0.03808
	TTG ⁻	1-3	1	a _i	3.75403	-0.85551	-1.50565	0.80569	-0.03285	0.01673	-0.00448
		OMe		b _i		3.26742	0.14743	0.18841	-0.19525	0.04198	-0.03902
	G ⁻ TG ⁺	2-5	1	a _i	0.38121	0.00000	0.00000	0.42315	0.00000	0.00000	0.04283
		Me		b _i		0.00000	0.00000	-0.01033	0.00000	0.00000	-0.00413
	G ⁻ TG ⁺	3-7	2	a _i	0.50933	0.00000	0.00000	0.53991	0.00000	0.00000	0.03020
		Me		b _i		0.00000	0.00000	-0.07562	0.00000	0.00000	-0.01732
	G ⁻ TG ⁺	1-2	1	a _i	4.18871	-0.15195	1.96255	0.47437	0.02270	-0.09508	-0.06642
		OMe		b _i		0.24178	2.49507	-0.10869	-0.08475	-0.07891	0.03000
	G ⁻ TG ⁺	1-3	2	a _i	2.37303	2.85666	-0.00024	0.67581	-0.13729	-0.05260	-0.04402
		OMe		b _i		1.58946	1.78286	0.23134	-0.12204	-0.03394	0.01172
	TTT	4-6	3	a _i	0.56546	-0.00035	0.00035	0.58698	0.00033	-0.00033	0.02855
		Me		b _i		-0.00003	0.00005	0.12042	0.00010	-0.00013	-0.01046
	TTT	1-4	3	a _i	3.64420	3.16516	0.29180	0.61767	-0.07037	-0.01082	-0.04904
		OMe		b _i		1.73775	1.33959	-0.05050	-0.08034	-0.07775	-0.01933
	A ⁺ A ⁺ G ⁺	2-5	1	a _i	0.26094	0.00000	0.00000	0.25957	0.00000	0.00000	0.00053
		Me		b _i		0.00000	0.00000	-0.00814	0.00000	0.00000	0.00090
	A ⁺ A ⁺ G ⁺	3-7	2	a _i	0.85603	0.00000	0.00000	0.88714	0.00000	0.00000	0.02749
		Me		b _i		0.00000	0.00000	-0.00861	0.00000	0.00000	-0.01174
	A ⁺ A ⁺ G ⁺	1-2	1	a _i	3.47186	0.26858	2.29482	0.50333	-0.03506	-0.07677	-0.06650
		OMe		b _i		-0.20451	2.99460	-0.22909	0.00789	-0.08930	0.04464

Species	Conform.	Rotor	#	Coef	i=0	i=1 (7)	i=2 (8)	i=3 (9)	i=4 (10)	i=5	i=6
	A ⁺ A ⁺ G ⁺	1-3	2	a _i	1.01621	0.16776	-0.61359	0.86939	0.01363	-0.01004	-0.02297
		OMe		b _i		-0.19825	0.55705	0.08959	-0.08029	0.01904	0.00138
2MMR	TG ⁻	2-5	1	a _i	0.65732	0.00000	0.00000	0.67568	0.00000	0.00000	0.02039
		Me		b _i		0.00000	0.00000	0.05888	0.00000	0.00000	-0.00430
	TG ⁻	3-6	1	a _i	0.71536	0.00000	0.00000	0.73749	0.00000	0.00000	0.01907
		Me		b _i		0.00000	0.00000	-0.01456	0.00000	0.00000	-0.01477
	TG ⁻	1-2	1	a _i	3.31615	2.11830	-0.63832	0.56775	0.07735	0.02852	-0.04222
		OMe		b _i		2.13173	2.09785	0.37705	-0.19561	-0.07906	0.00423
	TG ⁻	1-3	1	a _i	-0.30776	-0.46222	-0.32804	0.68421	-0.00367	0.00657	-0.00512
		OMe		b _i		-0.52660	-0.61905	-0.21344	0.05243	0.02928	-0.00112
	TT	2-5	2	a _i	0.78700	0.00000	0.00000	0.81879	0.00000	0.00000	0.02785
		Me		b _i		0.00000	0.00000	-0.00078	0.00000	0.00000	-0.01086
	TT	1-2	2	a _i	0.56541	-0.46222	-0.32804	0.68421	-0.00367	0.00657	-0.00512
		OMe		b _i		-0.52660	-0.61905	-0.21344	0.05243	0.02928	-0.00112
	TG ⁺	2-5	1	a _i	0.75493	0.00035	-0.00035	0.77544	-0.00035	0.00035	0.01976
		Me		b _i		0.00001	-0.00002	0.00035	-0.00003	0.00004	-0.01814
	TG ⁺	3-6	1	a _i	0.65157	0.00000	0.00000	0.61573	0.00000	0.00000	0.00807
		Me		b _i		0.00000	0.00000	-0.20732	0.00000	0.00000	0.01451
	TG ⁺	1-2	1	a _i	3.36740	3.24124	0.59733	0.62348	-0.10595	-0.04377	-0.04074
		OMe		b _i		-0.99181	-0.70774	-0.10125	-0.01036	0.01132	-0.02378
	TG ⁺	1-3	1	a _i	1.99945	-0.46222	-0.32804	0.68421	-0.00367	0.00657	-0.00512
		OMe		b _i		-0.52660	-0.61905	-0.21344	0.05243	0.02928	-0.00112
	A ⁻ G ⁻	2-5	1	a _i	0.69131	0.00000	0.00000	0.69692	0.00000	0.00000	0.01047
		Me		b _i		0.00000	0.00000	0.12865	0.00000	0.00000	0.01838
	A ⁻ G ⁻	3-6	1	a _i	0.58358	0.00000	0.00000	0.60928	0.00000	0.00000	0.02345
		Me		b _i		0.00000	0.00000	-0.05501	0.00000	0.00000	-0.01889
	A ⁻ G ⁻	1-2	1	a _i	1.56129	3.24124	0.59733	0.62348	-0.10595	-0.04377	-0.04074
		OMe		b _i		-0.99181	-0.70774	-0.10125	-0.01036	0.01132	-0.02378
	A ⁻ G ⁻	1-3	1	a _i	3.31615	2.11830	-0.63832	0.56775	0.07735	0.02852	-0.04222
		OMe		b _i		2.13173	2.09785	0.37705	-0.19561	-0.07906	0.00423
MMR		2-5	1	a _i	0.71536	0.00000	0.00000	0.72939	0.00000	0.00000	0.01737
		Me		b _i		0.00000	0.00000	0.06652	0.00000	0.00000	-0.00906
		1-2	1	a _i	1.87857	-0.49885	-2.26861	0.60577	0.77069	0.04866	-0.19074
		OMe		b _i		-0.02149	0.01296	-0.01409	0.01991	-0.04204	0.02899
2MER	G ⁺ G ⁺	1-4	1	a _i	0.86962	0.00000	0.00000	0.88285	0.00000	0.00000	0.01453
		Me		b _i		0.00000	0.00000	0.09104	0.00000	0.00000	-0.00182
	G ⁺ G ⁺	2-5	1	a _i	0.67091	0.00000	0.00000	0.60565	0.00000	0.00000	0.00896
		Me		b _i		0.00000	0.00000	-0.33235	0.00000	0.00000	-0.01619
	G ⁺ G ⁺	3-6	1	a _i	0.62646	0.00000	0.00000	0.60270	0.00000	0.00000	0.01664
		Me		b _i		0.00000	0.00000	-0.17691	0.00000	0.00000	0.02148
	G ⁺ G ⁺	1-2	1	a _i	2.95921	2.75891	0.86559	0.60753	-0.10341	-0.01581	-0.03553
		OMe		b _i		-0.44329	-1.29532	0.02877	-0.01431	-0.00012	-0.01041
	G ⁺ G ⁺	1-3	1	a _i	3.24221	-1.55459	-0.26769	0.65129	-0.00851	0.01124	-0.00658
		OMe		b _i		-1.17703	-0.61531	-0.33153	0.11188	0.03478	-0.03644
	TG ⁺	1-4	1	a _i	0.88584	0.00000	0.00000	0.93626	0.00000	0.00000	0.06548
		Me		b _i		0.00000	0.00000	0.26974	0.00000	0.00000	0.05155
	TG ⁺	2-5	2	a _i	0.62019	0.00000	0.00000	0.62853	0.00000	0.00000	0.05942
		Me		b _i		0.00000	0.00000	-0.23435	0.00000	0.00000	-0.01030
	TG ⁺	1-2	2	a _i	-0.52494	-1.55459	-0.26769	0.65129	-0.00851	0.01124	-0.00658
		OMe		b _i		-1.17703	-0.61531	-0.33153	0.11188	0.03478	-0.03644
	G ⁺ G ⁺	1-4	1	a _i	0.83250	0.00000	0.00000	0.62164	0.00000	0.00000	-0.00858
		Me		b _i		0.00000	0.00000	0.57385	0.00000	0.00000	0.01705
	G ⁺ G ⁺	2-5	1	a _i	0.57574	0.00000	0.00000	0.56016	0.00000	0.00000	0.01265
		Me		b _i		0.00000	0.00000	0.17293	0.00000	0.00000	-0.00340
	G ⁺ G ⁺	3-6	1	a _i	0.45913	0.00000	0.00000	0.48925	0.00000	0.00000	0.02878
		Me		b _i		0.00000	0.00000	0.02681	0.00000	0.00000	0.01990
	G ⁺ G ⁺	1-3	1	a _i	4.03136	0.39002	-0.70071	0.43199	0.08162	0.07916	-0.02351

Species	Conform.	Rotor	#	Coef	i=0	i=1 (7)	i=2 (8)	i=3 (9)	i=4 (10)	i=5	i=6
		OMe		b _i		-2.60917	-1.61568	-0.50061	0.18144	0.05026	-0.00673
	G ⁺ G ⁺	1-2	1	a _i	1.63146	2.75891	0.86559	0.60753	-0.10341	-0.01581	-0.03553
		OMe		b _i		-0.44329	-1.29532	0.02877	-0.01431	-0.00012	-0.01041
MPR		1-3	1	a _i	0.92174	-0.00014	0.00023	0.92002	0.00004	-0.00030	0.03537
		Me		b _i		-0.00032	-0.00026	0.29836	0.00035	0.00017	0.04144
		1-4	1	a _i	0.72950	0.00000	-0.00003	0.52283	0.00002	0.00003	0.00158
		Me		b _i		-0.00003	-0.00002	-0.52194	0.00003	-0.00001	-0.00845
		2-5	1	a _i	0.98292	0.00035	-0.00034	0.92877	-0.00031	0.00029	0.00166
		Me		b _i		-0.00004	0.00008	-0.39426	0.00015	-0.00019	-0.03397
		1-2	1	a _i	1.64293	-0.48712	-1.99114	0.71478	0.57297	-0.09274	-0.06578
		OMe		b _i		0.00412	-0.06106	0.02223	0.04362	-0.00441	-0.01634
MER	T	1-3	1	a _i	0.95905	0.00000	0.00000	1.03590	0.00000	0.00000	0.04427
		Me		b _i		0.00000	0.00000	-0.04124	0.00000	0.00000	-0.02876
	T	2-5	1	a _i	0.93394	0.00000	0.00000	0.95826	0.00000	0.00000	0.03754
		Me		b _i		0.00000	0.00000	0.12688	0.00000	0.00000	-0.00650
	T	1-2	1	a _i	0.71270	0.83005	-1.70425	0.51381	0.67034	0.14673	-0.14546
		OMe		b _i		-0.03053	-0.05405	0.02700	0.10442	-0.01787	-0.12482
	C	1-3	1	a _i	0.66935	0.00000	0.00000	0.61291	0.00000	0.00000	0.00379
		Me		b _i		0.00000	0.00000	0.26562	0.00000	0.00000	-0.00167
	C	2-5	1	a _i	0.73820	0.00035	-0.00035	0.74885	-0.00034	0.00034	0.01556
		Me		b _i		-0.00001	0.00003	-0.07554	0.00005	-0.00007	0.00385
	C	1-2	1	a _i	2.62412	0.83005	-1.70425	0.51381	0.67034	0.14673	-0.14546
		OMe		b _i		-0.03053	-0.05405	0.02700	0.10442	-0.01787	-0.12482